PHYSICAL CHEMISTRY

TARGET CSIR NET | IIT GATE

QUANTUM CHEMISTRY

DPP :- 1-20

Address -"Quanta Chemistry Classes, 50 Mall Road, near GTB nagar metro station, Gate no 3,

Kingsway Camp, GTB Nagar, New Delhi (110009) INDIA".

Tel.:9990382567, 9717373074, 8285815185

Email: Quantachemistryclasses@gmail.com

Website :www.quantachemistryclasses.com

QUANTA POINT

DPP- (1) Quantum Chemistry

1. The value of A^2 [if $A = x - (d/dx)$] is

(a) $x^2 + (d^2/dx^2) - 2x\,(d/dx)$ (b) $(d^2/dx^2) - 2x\,(d/dx) + x^2 - 1$

(c) $-(d^2/dx^2) - 2x(d/dx) + x^2 - 1$ (d) $x^2 + (d^2/dx^2) - 2x(d/dx) + 1$

2. Consider the statement

(i) "SQRT" operator is Linear operator

(ii) An operator is linear if $A(f+g) = Af + Ag$ (A is operator f and g is the function)

(iii) In quantum mechanics operator used must be linear.

The Correct statement above are

(a) (i) (b) (ii) (c) (iii) (d) (ii) and (iii)

3. Two different non zero operator A and B $(A \neq B)$ satisfy the relation $(A+B)(A-B) = A^2 - B^2$ when

(a) $AB = A^2$ and $BA = B^2$ (b) $AB + BA = 0$

(c) A and B are arbitary (d) $AB - BA = 0$

4. The value of commutator (x^3, p_x) is equal to

(a) x^2 (b) $-3x^2 i\hbar$ (c) $+3x^2 i\hbar$ (d) zero

5. Consider the statement

(i) If A is linear operator then the value of $[Af(x)]^2 \neq A^2 f(x)$

(ii) The value of commutator $[x,(x,p_x^2)]$ is equal to 0.

(iii) The multiplication of two linear operator is linear.

(iv) Square root is not linear operator but square is a linear operator

The correct statements above are

(a) (i) and (iii) (b) (ii) and (iv) (c) (i),(ii),(iii) (d) (iii) only

6. Consider the statement

(i) The commutator of d/dx with x is a unit operator.

(ii) Differentiation and integration operator are linear because for being a linear operator $A\{C_1 f_1(x) + C_2 f_2(x)\} = C_1 A f_1(x) + C_2 A f_2(x)$ is the condition

(iii) Linear operator always commute with any number.

The correct statement above are

(a) (i) and (ii) (b) (ii) and (iii) (c) (i), (ii) and (iii) (d) None

QUANTA POINT

7. Evaluate the commutator {x, d/dx} operating on arbitary wave function f(x)

(a) 0 (b) –1 (c) +1 (d) ∞

8. The value of [x, p_x] is equal to

(a) 0 (b) $\hbar / i$ (c) $-i\hbar$ (d) $-\hbar / i$

9. The value of the commutator [x, [x, p_x]] is

(a) $i\hbar x(2) - i\hbar$ (b) $-i\hbar$ (c) $i\hbar$ (d) 0

10. The operator [x,[x,p^2]] is identical with

(a) [px, [x,p]] (b) [xp,[x,p]] (c) –[p,[x^2,p]] (d) [x,[x^2,p]]

11. The value of commutator (1/x, p_x)

(a) $-(h / 2\pi i)x^2$ (b) $(h / 2\pi i)x^2$

(c) $(h / 2\pi i)\, x^2$ (d) $-(h / 2\pi i)\, x^2$

12. The value of commutator (x, p_x^2) is given by

(a) $2\, ih / \pi$ (b) $(h^2 / 2\pi^2)\,(d / dx)$

(c) $(h^2 / 4\pi^2)\,(d / dx)$ (d) $-(h^2 / 2\pi^2)(d / dx)$

13. When the operator $-\left(\hbar^2 / 2m\right)\left(d^2 / dx^2\right)$ operates as a function e^{-ikx}

(a) $k^2\hbar^2 e^{-ikx}$ (b) $i\, k^2\hbar^2 e^{-ikx}$

(c) $i\hbar^2 e^{-ikx}$ (d) $\hbar^2 e^{-ikx}$

14. Denote the commutator of two matrices A and B by [A,B] = AB – BA ; the anti-commutator {A, B} = AB + BA

(a) –B[A, C] (b) B[A, C]

(c) –B{A, C} (d) [A, C]B

15. The commutator of x with Hamiltonian H, $\left[x, H_x\right]$ is

(a) 0 (b) i (c) $-\left(\hbar^2 / 2m\right) p_x$ (d) $(i\,\hbar / m)\, p_x$

×××××

QUANTA POINT

DPP- (2) Quantum Chemistry

1. The linear momentum of a particle described by the wave function e^{-ikx} is

   (a) kh (b) $-kh$ (c) $k\hbar$ (d) $-k\hbar$

2. The commutator of kinetic energy operator T_x and the momentum operator px for the one dimensional case is

   (a) $(ih/2\pi)$ (b) $(ih/2\pi)(d/dx)$

   (c) 0 (d) $(ih/2\pi)x$

3. The operation of commutator [x, d/dx] on a function f(x) is equal to

   (a) 0 (b) f(x) (c) –f(x) (d) x, df/dx

4. Which of the following pairs of operator commute

   (a) x and (d/dx) (b) (d/dx) and $(d^2/dx^2)+2(d/dx)$

   (c) $x^2(d/dx)$ and (d^2/dx^2) (d) x^3 and (d/dx)

5. The value of $[x, p_y]$, $[p_x, p_y]$ respectively are (arbitary function state function)

   (a) 0, 0 (b) 0, not zero (c) not zero (d) not zero, not zero

6. The "SQRT and SQR" operator

   (a) Commute with each other (b) do not commute with each other

   (c) cannot determine (d) None of these

7. The value of commutator (x^2, p_x^2) is equal to

   (a) $(ih/2\pi)(xp_x + p_x x)$ (b) $(ih/\pi)(xp_x + p_x x)$

   (c) 0 (d) $2ih/\pi$

8. The operators $S_{\pm}$ are defined by $S_{\pm} = S_x \pm iS_y$, where S_x and S_y are component of the spin angular momentum operator. The commutator $[S_z, S_+]$ is

   (a) $\hbar S_-$ (b) $\hbar S_+$ (c) $-\hbar S_+$ (d) $-\hbar S_-$

9. Consider the statement

   (i) The value of $\{x, L_x\}$ is 0

   (ii) The value of comutator {x, y} is z

QUANTA POINT

(iii) If two operator commute they have common set of eignfunction.

The correct statement above are

(a) i, ii (b) iii and ii (c) i, iii (d) none

10. The value of [A[B, C]] + [B, [C,A]] + [C, [A, B]] is equal to

(a) 1 (b) –1 (c) 0 (d) ∞

11. The value of commutator $[L_y, p_z]$

(a) $(ih/2\pi)p_y$ (b) $(ih/2\pi)p_z$ (c) 0 (d) $(ih/2\pi)p_x$

12. The operator $L_{\pm} = L_x \pm iL_y$ where L_x and L_y are the x and y component of angular momentum. The commutator $[L_z, L_-]$ is

(a) $hL_+/2\pi$ (b) $hL_-/2\pi$ (c) $-hL_+/2\pi$ (d) $-hL_-/2\pi$

13. Given operator $a_+ = \frac{1}{\sqrt{2}}(x + ip_x)$ and $a_- = \frac{1}{\sqrt{2}}(x - ip_x)$ where x and p_x are the positon and linear momentum operator, respectively the value of commutator $[a_+, a_-]$ is equal to

(a) $ih/2\pi$ (b) $-ih/2\pi$ (c) $h/2\pi$ (d) $-h/2\pi$

××××

QUANTA POINT

DPP- (3) Quantum Chemistry

1. The vlaue of commutator $\{x, p_x\}$ is

   (a) 0 (b) $(ih/2\pi)$ (c) $(ih/2\pi)(d/dx)$ (d) x

2. Find the value of commutator $\{x^2, d^2/dx^2\}$.

   (a) –1 (b) –2 (c) 4 (d) None

3. The value of commutator $\{x, p_x^2\}$ is given by

   (a) $2ih/\pi$ (b) $(h^2/2\pi^2)(d/dx)$

   (c) $(h^2/4\pi^2)(d/dx)$ (d) $-(h^2/2\pi^2)(d/dx)$

4. If operator d^n/dx^n is operated on function $e^{\alpha x}$ then the result is

   (a) α^n (b) $\alpha^n e^{\alpha x}$ (c) $e^{\alpha x}$ (d) α

5. Consider the statements

   (i) $i\{A + A^+\}$ is an antihermitian and $i\{A - A^+\}$ is hermitian

   (ii) xp_x is not hermitian but $xp_x + p_x x$ is hermitian

   (iii) the commutator of x with p_y is 0 but L_x with p_y is non-zero

   (a) i, ii (b) ii, iii (c) i, ii, iii (d) iii only

6. Consider the statement :

   (i) If A is hermitian B is hermitian then [AB + BA] is hermitian but [AB– BA] is antihermitian

   (ii) If A is hermitian B is hermitian then i{A + B} is antihermitian and i[A – B] is hermitian

   (iii) The multiplication of two commuating hermitian operator is hermitian

   The correct statements above are

   (a) i only (b) i, ii (c) ii only (d) iii and i

7. Identify which of the following operator is not hermitian

   (a) $(h/2\pi i)(d/dx)$ (b) (id^2/dx^2) (c) (d^2/dx^2) (d) x^2

8. Consider the statements :

   1. $(A + A^+)$ is hermitian and $(A - A^+)$ is antihermitian

   2. $K_x p_x$ and $K_x + p_x$ is hermitian operator

   3. The operaor $L_x L_y + L_y L_x$ is Hermitian operator.

   The correct stastements above are

   (a) 1, 2 (b) 2, 3 (c) 1, 2, 3 (d) 1, 3 (e) none

QUANTA POINT

9. Given two hermitian opeator A and B we construct four operator AB, ABA, i[A,B], A^2B. Choose the correct option from below:

(a) All these four operators are Hermitian

(b) Only three of these are hermitian in nature

(c) Only two of these are hermitian in nature

(d) Only one of these operator is hermitian

10. The hermitian conjugate of d/dx is

(a) d/dx (b) – d/dx (c) x (d) 0

11. Consider the statement

(i) Hermitian operator always commute with one another

(ii) Hermitian operator always have real eigenvalues

(iii) The multiplication of two hermitian operator is hermitian

The correct statements above are

(a) (i) only (b) (i), (ii) (c) (ii) only (d) (iii) only

12. Consider the statement :

(i) If A is hermitian B is hermtian then {AB + BA} is hermitian but {AB – BA} is antihermitian

(ii) If A is hermitian B is hermitian, i{A + B} is antihermitian and i{A – B} is hermitian

(iii) The mulitplication of two commutating hermitian operator is hermitian

The correct statements above

(a) (i) only (b) (i), (ii) (c) (ii) only (d) (iii) only

13. If operator A = –(d/dx) + x then

(a) A is hermitian (b) A is anti-hermitian

(c) $A\,A^{\dagger}$ is hermitian (d) $A\,A^{\dagger}$ is anti-hermitian

14. If an operator $\left\{d^2/dx^2 - 16x^2\right\}$ is operated on an function e^{-2x^2} than corresponding eigen value is

(a) 2 (b) –4 (c) 2 (d) 4 (e) none

15. When the operator $-\left(\hbar^2/2m\right)\left(d^2/dx^2\right)$ operates on a function e^{-ikx} the result is

(a) $\frac{k^2\hbar^2}{2m}e^{-ikh}$ (b) $\frac{ik^2\hbar^2}{2m}e^{-ikx}$ (c) $\frac{i\hbar^2}{2m}e^{-ikx}$ (d) $\frac{\hbar^2}{2m}e^{-ikx}$

××××

QUANTA POINT

DPP- (4) Quantum Chemistry

1. If $\hat{L}_x, \hat{L}_y, \hat{L}_z$ are the components of the angular momentum operator in three dimensions the commutator $\left[\hat{L}_x, \hat{L}_x\hat{L}_y\hat{L}_z\right]$ may be simplified to

   (a) $i\hbar L_x\left(\hat{L}_z^2 - \hat{L}_y^2\right)$ (b) $i\hbar\hat{L}_z\hat{L}_y\hat{L}_x$ (c) $i\hbar L_x\left(2\hat{L}_z^2 - \hat{L}_y^2\right)$ (d) 0

2. If L_x, L_y and L_z are respectively the x ,y and z components of angular momentum operator L. The commutator $\left[L_x L_y, L_z\right]$ is equal to

   (a) $i\hbar\left(L_x^2 + L_y^2\right)$ (b) $2i\hbar L_z$ (c) $i\hbar\left(L_x^2 - L_y^2\right)$ (d) 0

3. The linear momentum of a particle decribed by the wavefunction e^{-ikx} is

   (a) kh (b) – kh (c) $-kh/2\pi$ (d) $kh/2\pi$

4. Consider the statements

   (i) the expectation value of a Hermitian operator is real and that of an anti-Hermitian operator is imaginary

   (ii) anticommutator {A, B} is defined by AB-BA

   (iii) Hermitian conjugate of a commutator is $\left[\hat{A},\hat{B}\right]^{\dagger} = \left[\hat{B}^{\dagger},\hat{A}^{\dagger}\right]$

   The correct statement above are

   (a) (i) (b) (i), (ii) (c) (i), (iii) (d) (i)

5. The correct statement among the following is (A is hermitian operator)

   (a) The eigen value of A^2 can be negative

   (b) The eigen value of A^2 are always positive

   (c) No eigenfunction of A is an eignfunction of A^2

   (d) The eignvalue of A^2 can be complex

6. Which of the following is common eignfunction of d/dx and d^2/dx^2 operators

   (a) cos x (b) kx (c) e^{ix} (d) $e - x^2$

7. For a hermitian operator A, which does not commute with the Hamiltonian H, let ψ_1 be an eignfunction of A and ψ_2 be an eignfunction of H. The correct statement regarding the average value of commutator of A with H([A,H]) is

   (a) both $<\psi_1\left[A,H\right]\psi_1>$ and $<\psi_2\left[A,H\right]\psi_2>$ are non zero

   (b) only $<\psi_1\left[A,H\right]\psi_1>$ is zero, but $<\psi_2\left[A,H\right]\psi_2>$ is non zero

   (c) only $<\psi_2\left[A,H\right]\psi_2>$ is zero, but $<\psi_1\left[A,H\right]\psi_1>$ is non zero

   (d) Both $<\psi_1\left[A,H\right]\psi_1>$ and $<\psi_2\left[A,H\right]\psi_2>$ are zero

QUANTA POINT

8. A set of N vectors $X_1, X_2 \ldots\ldots X_n$ satisfy the eigenvalue equation for an operator A with scalar eigenvalues $\lambda_1, \lambda_2, \ldots\ldots \lambda_n$ (i.e., $AX_k = \lambda_k X_k$). The linear combination of vector $X = \in C_k X_k$, where C_k are non-zero scalar coefficient.

(a) is not an eigenvector of A

(b) is an eigenvector of A only if the λ_k are all distinct (no two eigenvalues are equal)

(c) is an eigenvector of A only if the λ_k are all equal

(d) is an eigenvector of only if C_k are equal

9. The eigenfunctions of the Hamiltonian H (H = T + V) of a harmonic oscillator are (where T and V are kinetic energy and potential energy operators respectively)

(a) eigenfunctions of T as well as V

(b) eigenfunctions of T, but not of V

(c) eigenfunctions of V but not of T

(d) eigenfunctions of neither T nor V

10. Which of the following statement is not true

(i) The state function $\psi(x,t)$ is always equal to a function of time multiplied by a function of coordinate.

(ii) If f_1 and f_2 are eign functions of operator B then $C_1 f_1 + C_2 f_2$ must always be an eignfunction of B, where C_1 and C_2 are constants

(iii) The operator L^2 commute with $L_x + L_y$.

(a) (i), (iii) (b) (i), (ii) (c) (ii), (iii) (d) only (iii)

11. When the operator $-(\hbar^2)(d^2/dx^2)$ operates on a function e^{-ikx} the result is

(a) $k^2\hbar^2 e^{-ikx}$ (b) $ik^2\hbar^2 e^{-ikx}$ (c) $i\hbar^2 e^{-ikx}$ (d) $\hbar^2 e^{-ikx}$

12. If an operator $\{(d^2/dx^2) - 16x^2\}$ is operated on an function e^{-2x^2} than corresponding eigenvalue is

(a) –2 (b) –4 (c) 2 (d) 4

13. $\{(-h^2/8\pi^2 m)(d^2/dx^2) + (h^2\alpha^2x^2)/2\pi^2 m\} e^{-\alpha x^2} = C(h^2/4\pi^2) e^{-\alpha x^2}$ $(h, \pi, \alpha, m \text{ constant})$, value of C is

(a) $2\alpha/m$ (b) $\alpha/2m$ (c) α/m (d) α^2/m

14. The probability of finding the particle in a one of dimensional box of length 'L' in the region between $\frac{L}{4}$ and $\frac{3L}{4}$ for quantum number n = 1 is

(a) $\frac{1}{2}$ (b) $\frac{1}{2} + \frac{1}{\pi}$ (c) $\frac{1}{2} - \frac{1}{\pi}$ (d) $\frac{2}{3}$

15. <x> in the ground state for a particle that is confined to move in a one d box of length -L to L is

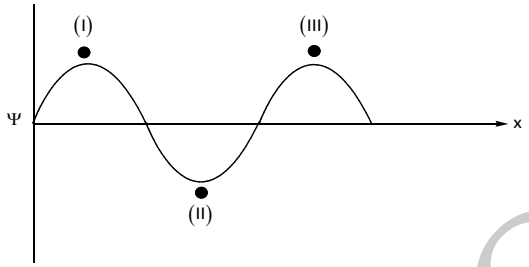
(a) L (b) L/2 (c) –L (d) 0

××××

QUANTA POINT

DPP- (5) Quantum Chemistry

1. A system is described by the following real wavefunction. The probability (P) of finding the particle in a region dx around point I, II and III in the figure obeys the trend



(a) P(I) >P(II) >P(III)
(b) P(II) > P(III) > P(I)
(c) P(II) >P(I) >P(III)
(d) P(III) > P(I) > P(II)

2. Consider a particle of mass m moving n a one dimensional box under the potential V = 0 for $0 < x < a$ and V= infinite outside the box. When the particle is in lowest energy state, the average momentum $< p_x >$ of the particle is

(a) $< p_x > = 0$
(b) $< p_x > = (h/a)$
(c) $< p_x > = (h/2a)$
(d) $< p_x > = \left(h / 2\pi a\right)$

3. The uncertainty in the momentum Δp_x of the particle in its lowest energy state is

(a) $\Delta p_x = 0$
(b) $\Delta p_x = (h / a)$
(c) $\Delta p_x = (h / 2a)$
(d) $\Delta p_x = (h / 2\pi a)$

4. For a particle of mass m confined in a box of length L, assume $\Delta x = L$. Assume further that $\Delta p_{min} = < p^2 >^{1/2}$. Use the uncertainty principle to obtain an estimate of energy of the particle the value will be

(a) $h^2/8mL^2$ (b) $h^2/8mL^2$ (c) $h^2/32mL^2$ (d) $h^2/2mL^2$

5. Suppose, the ground stationery state of a harmonic oscillator with force constant 'k' is given $\Psi_0 = \exp\left[-Ax^2\right]$. Then, A should depend on k as

(a) $A \propto k^{-1/2}$ (b) $A \propto k$ (c) $A \propto k^{1/2}$ (d) $A \propto k^{1/3}$

6. Given three systems, A, B, and C, what could be they if the spacing between neighbouring energy levels in A decreases with increasing energy, while that for B is constant, and that for C increases with increasing energy?

QUANTA POINT

(a) A = particle in 1D box, B = harmonic oscillator, C = electron in hydrogen atom

(b) A= electron in hydrogen atom, B = harmonic oscillator, C = particle in a 1D box

(c) A= particle in a 1D box B = electron in hydrogen atom, C = harmonic oscillator

(d) A = electron in hydrogen atom, B = particle in a 1D box, C = harmonic oscillator

7. The Mathematical expression $e^{i(kx-wt)}$ represents

(a) a wave stationary in space but oscillating in time

(b) a travelling wave moving in the positive x direction

(c) a wave stationary in time but periodically varying in space

(d) a travelling wave moving in the negative x direction

8. The unit of wave function corresponding to particle confined to move in 1D box is

(a) $L^{½}$ (b) $L^{-½}$

(c) L (d) dimensionless

9. The lowest allowed energy is equal to zero for

(a) the hydrogen atom (b) rigid rotor

(c) a harmonic oscillator (d) a particle in 3D box

10. The energy of second excited state of the hydrogen atom is

(a) –27.2 eV (b) – 6.8 eV (c) –1.5 eV (d) –4.5 eV

11. Determine the probability of finding the particle between L/4 to 3L/4 for a particle in 1Dbox of length $(0 < x < L)$ in the first excited state

(a) 1/4 (b) 1/3 (c) 1/2 (d) 1

12. For hydrogen-like atom with a nuclear charge Z, the energy of orbtial with principal quantum number 'n' follows the relation.

(a) $E_n \propto n^2Z^2$ (b) $E_n \propto Z^2/n^2$ (c) $E_n \propto Z^2/n$ (d) $E_n \propto n^2/Z^2$

13. For the particle in a box problem in (0, L), the value of $\langle x^3 \rangle$ in the $n \to \infty$ would be

(a) $L^3/6$ (b) $L^3/3$ (c) $L^3/4$ (d) $L^4/4$

14. For a hydrogen atom, which of the following orbital(s) have the lowest energy?

(a) 4*s* (b) 4 *p*

(c) 4*d* (d) All of these have same energy

15. The value of commutator [Sin x, d/dx] is equal to

(a) Cos x (b) –Cos x (c) tan x (d) 0

16. When we operate the operator $-x^2(\delta/\delta x)$ on the function e^{-3x} the corresponding eigen value

(a) –3 (b) +3 (c) –1 (d) None

QUANTA POINT

17. The energy of 2S orbital and 2*p* orbitalis same for

(a) Li (b) Li^{2+} (c) Be^{2+} (d) H^{+}

18. The wave function for a quantum mechanical particle in a 1 dimensional box of length 'a' is given by $\psi = A\sin(\pi x / a)$. The value of A for a box of length 200 nm is

(a) $4 \times 10^4\ (nm)^2$ (b) $10\sqrt{2}\ (nm)^{1/2}$ (c) $\sqrt{2}/10\ nm^{-1/2}$ (d) $0.1\ nm^{-1/2}$

19. A very general form of the uncertainity principle was developed by H.P. Robertson in 1929 for two observables A and B is

(a) $\Delta A\,\Delta B > \{0.5 < [A,B] >\}$ (b) $\Delta A\,\Delta B > \{0.5[A,B]\}$

(c) $\Delta A\,\Delta B < \{0.5 < [A,B] >\}$ (d) $\Delta A\,\Delta B < \{0.5[A,B]\}$

20. Consider the statement

(i) If g is an eigen function of the linear operator B, then cg is an eigen function of B, where c is an arbitary constant

(ii) For a stationary state, the probability density is independent of time

(iii) If f is an eigen function of the linear opeator A with eigen value a, then f is an eigen function of A^2 with eigen value a^2

The correct statement above is/are

(a) (i) (b) (i), (ii) (c) (i), (ii), (iii) (d) (i), (iii)

QUANTA POINT

DPP- (6) Quantum Chemistry

1. The value of deviation in the radius $\langle r^2\rangle - \langle r\rangle^2$ in the 1s state of hydrogen atom is (a_0 Bohr radius)
   (a) a_0^2 (b) $1.5\,a_0^2$ (c) $0.75\,a_0^2$ (d) $0.5\,a_0^2$
2. The average value of the radus $\langle r\rangle$ in the 1s state of hydrogen atom is (a_0 Bohr radius)
   (a) a_0 (b) $1.5a_0$ (c) $0.75a_0$ (d) $0.5a_0$
3. The ionization energy of hydrogen atom in the ground sate is approximately 13.6 eV. The potential energy of He^+, in its ground state is approximately
   (a) –54.4 eV (b) –27.2 eV (c) –13.6 eV (d) –108.8 eV
4. The ground state energy of hdrogen atom is –13.598 eV. The expectation value of kinetic energy $\langle T\rangle$ and potential energy $\langle V\rangle$, in unit of eV is
   (a) $\langle T\rangle$ = 13.598 eV, $\langle V\rangle$ = –27.196 eV (b) $\langle T\rangle$ = –27.196 eV, $\langle V\rangle$ = 13.598 eV
   (c) $\langle T\rangle$ = –6.799 eV, $\langle V\rangle$ = –6.799 eV (d) $\langle T\rangle$ = 6.799 eV, $\langle V\rangle$ = –20.397 eV
5. Consider the statements
   (i) The energy corresponding to 2*s* orbital of hydrogen atom is –0.125 a.u.
   (ii) The energy of hydrogenic atom is directly proportional to μZ^2
   (iii) The energy of 2*s* and 2*p* orbital of hydrogenic species is equal they are degenerate according to Schrodinger equation
   Correct statement above are
   (a) (i), (ii) (b) (ii), (iii) (c) (i), (iii) (d) (i), (ii), (ii) (e) none
6. Which of the following statement is / are true
   (i) The state function $\psi(x,t)$ is always equal to a function of time multiplied by a function of coordinate
   (ii) If f_1 and f_2 are eigen functions of operator B then $C_1f_1 + C_2f_2$ must always be an eigen function of B, where C_1 and C_2 are constants
   (iii) The operator L^2 commute with $L_x + L_y$
   (a) (i), (iii) (b) (i), (ii) (c) (ii), (iii) (d) only (iii)
7. For a harmonic oscillator in its ground state i.e., v = 0 state, the energy is given by $E_0 = (1/2)hv$ where v is the vibrational energy. This is due to its
   (a) Kinetic energy (b) Potential energy
   (c) Heat of formation (d) Sum of Kinetic and potential energy
8. Two bound stationary states, 1 and 2 of a one electron atom with $E_2 = E_1$ (E is the toal energy) obey the following statement about their kinetic energy (T) and potential energy (V)
   (a) $T_2 > T_1$; $V_2 > V_1$ (b) $T_2 > T_1$; $V_2 > V_1$ (c) $T_2 < T_1$; $V_2 > V_1$ (d) $T_2 = T_1$; $V_2 > V_1$

QUANTA POINT

9. Consider the statement

1. Virial Theorem are applicable to atom and molecule both.

2. According to virial energy contributed by potential and kinetic energy are equal.

3. For first excited state in SHO the energy contributed by kinetic energy is 75 hv

Correct statements abvoe are

(a) 1, 2 (b) 2, 3 (c) 1, 3 (d) 1, 2, 3 (e) none

10. Normalization constant for an electron in an orbtial of hydrogen atom with the wavefunction $\psi = e^{-r}$ is

(a) $1/2\sqrt{\pi}$ (b) $1/\sqrt{\pi}$ (c) $2/\sqrt{\pi}$ (d) 2

11. Average value of z coordinate for an electron in 1*s* orbital of hydrogen atom is

(a) $1.5a_0$ (b) a_0 (c) $2a_0$ (d) 0

12. For the eigenstate of hydrogen atom, which of the following relation between expectation value of kinetic energy <T> and potental energy <V> is given by

(a) <T> =<V> (b) 2<T> = – <V> (c) 2<T> = <V> (d) <T> = –2<V>

13. The unit of wavefunction ψ of hydrogen atom is

(a) L^3 (b) L^{-3} (c) $L^{-3/2}$ (d) dimensionless

14. Uncertainity in momentum for an electron in 1*s* obrital of hydrogen atom is

(a) $h/2\pi a_0$ (b) h/a_0 (c) $h/\pi a_0$ (d) 0

15. Electron is in the ground state of a hydrogen atom. The probability that it is within the Bohr radius is approximately equal to

(a) 0.60 (b) 0.90 (c) 0.16 (d) 0.32

QUANTA POINT

DPP- (7) Quantum Chemistry

1. The correct statement about both the average value of position <x> and momentum <p> of a 1-d haromonic oscilator wavefunction is

(a) $\langle x\rangle = 0, \langle p\rangle \neq 0$ (b) $\langle x\rangle \neq 0, \langle p\rangle \neq 0$ (c) <x> = 0, <p> = 0 (d) $\langle x\rangle \neq 0, \langle p\rangle = 0$

2. The wavefunction of a 1D harmonic oscillator is given as

$\psi(x) = N(2x^2 - 1)e^{x^2/2}$. The value of N that normalizes the function $\psi(x)$ is

$$\left(\text{Given: } \int_{-\infty}^{+\infty} x^{2n} e^{x^2} dx = \frac{1.3.5....(2n-1)}{2^n}\sqrt{\pi}\right)$$

(a) $\left(\frac{1}{8\sqrt{\pi}}\right)^{1/2}$ (b) $\left(\frac{1}{3\sqrt{\pi}}\right)^{1/2}$ (c) $\left(\frac{1}{2\sqrt{\pi}}\right)^{1/2}$ (d) $\left(\frac{1}{4\sqrt{\pi}}\right)^{1/2}$

3. For an one-dimensional quantum-mechanical harmonic oscillator

(a) Average linear momentum is non zero but average displacement is zero

(b) Average linear momentum is zero and average displacement is zero

(c) Average linear momentum is zero but average displacement is non zero

(d) Average linear momentum is and average displacement both are non zero

4. Consider the statement

(1) Virial theorem are applicale to atom and molecule both

(2) Accordng to virial energy contributed by potential energy and kinetc energy are equal

(3) For first excited state in SHO the energy contributed by kinetic energy is 7.5 hv

Correct statements above are

(a) 1.2 (b) 2.3 (c) 1.3 (d) 1, 2, 3

5. An electron of mass 'm' is confined to a one dimensional box of length 'b'. If it makes a radiative transition from second exicted state to the ground state the frequency of photon emitted as

(a) $9h / 8mb^2$ (b) $3h / 8mb^2$ (c) h/mb^2 (d) $2h / mb^2$

QUANTA POINT

6. A particle is confined to move in 1D box of length 1 mm. If the length is changed by 10^{-9} m, the percentage change in ground state energy is

(a) 2×10^{-4} (b) 2×10^{-7} (c) 2×10^{-2} (d) 0

7. The probability of finding the particle in one dimensional box of length L, in the region between L/4 and 3L/4 for quantum number n = 1 is

(a) 1/2 (b) $(1/2)+(1/\pi)$ (c) $(1/2)-(1/\pi)$ (d) 2/3

8. For a particle undergoing quantum mechanical tunneling

(i) the amplitude of the wavefunction after passing through the barrier decreases with increases in width

(ii) Tunneling barrier height increases the tunneling probability decreases

(iii) The energy of the particle after the crossing decreases with increases in distance

The correct statement above are

(a) (i), (ii) (b) (ii), (iii) (c) (i), (iii) (d) (i), (ii), (iii)

9. The zero point energy of a particle of mass m confined to move in a one dimensional box of length l is

(a) 0 (b) $\hbar^2\pi^2/mL^2$ (c) $\hbar^2\pi^2/2mL^2$ (d) $3\hbar^2\pi^2/2mL^2$

10. The transmission probability of a particle encountering the barrier is e^{-10} if mass is reduced by 1/2 and width of the barrier is doubled, tunneling probability would be

(a) $e^{-10\sqrt{2}}$ (b) e^{-20} (c) $e^{-20\sqrt{2}}$ (d) does not change

××××××

QUANTA POINT

DPP- (8) Quantum Chemistry

1. The degeneracy of quantum mechanical particle of a cubic box having energy two times than the group state energy is

   (a) 3 (b) 6 (c) 1 (d) 4

2. A particle in 3d cubic box of length *l* has the energy $14h^2/8ml^2$. The degeneracy of the state is

   (a) 2 (b) 3 (c) 6 (d) 9

3. A particle of a mass m is in a cubic box of side a. The potential inside the box $(0 \le x < a, 0 \le y < a, 0 \le z < a)$ is zero and infinite outside. If the particle is in an eigenstate of energy $14\hbar^2\pi^2 / 2ma^2$ its wavefunction is

   (a) $\psi = (2/a)^{3/2} \sin(3\pi x/a)\sin(5\pi y/a)\sin(6\pi z/a)$

   (b) $\psi = (2/a)^{3/2} \sin(7\pi x/a)\sin(4\pi y/a)\sin(3\pi z/a)$

   (c) $\psi = (2/a)^{3/2} \sin(4\pi x/a)\sin(8\pi y/a)\sin(2\pi z/a)$

   (d) $\psi = (2/a)^{3/2} \sin(\pi x/a)\sin(2\pi y/a)\sin(3\pi z/a)$

4. The degeneracy corresponding to quantum mechanical particle in a 3Dbox of length 'a' with energy E = $33\hbar^2\pi^2 / mL^2$ is

   (a) 6 (b) 8 (c) 12 (d) 14

5. A particle is confined in a 1D box of length 2a with potential v = infinite x < –a, x > a and v = 0 inside the box. Energy difference between the level n = 3 and n = 2 is

   (a) $5h^2/8ma^2$ (b) $9h^2/8ma^2$

   (c) $9h^2/32ma^2$ (d) $5h^2/32ma^2$

6. The wavelength associated with particle in a one dmensional box of length *l* is (n refers to quantum number)

   (a) 2*l*/n (b) *l*/n (c) n*l* (d) *l*/2n

7. A particle is in the ground state of an infinite square well potential given by, V = 0 inside the box –a < x < a and v = infinite otherwise. The probability to find the particle in the interval between –a/2 and a/2 is

   (a) 1/2 (b) $(1/2) - (1/\pi)$ (c) $(1/2) + (1/\pi)$ (d) $1/\pi$

8. A particle is in one-dimensional box with a potential V_0 inside the box and infinite outside. An energy state corresponding to n = 0(n : quantum number) is not allowed because

   (a) The total energy becomes zero

   (b) The average momentum becomes zero

   (c) The wavefunction becomes zero everywhere

   (d) The potential $V_0 = 0$

QUANTA POINT

9. A paricle of mass m is confined in the ground state of one dimensional box extending from –2L to +2L the wave function of particle in box is $\psi = \psi_0 \cos(\pi x / 4L)$ where ψ_0 is constant

(i) The normalization constant ψ_0 of the function is

(a) $(2/L)^{0.5}$ (b) $(1/4L)^{0.5}$ (c) $(1/2L)^{0.5}$ (d) $(1/L)^{0.5}$

(ii) The energy eigenvalue corresponding to this state is

(a) $\hbar^2\pi^2/2mL^2$ (b) $\hbar^2\pi^2/4mL^2$ (c) $\hbar^2\pi^2/16mL^2$ (d) $\hbar^2\pi^2/32mL^2$

(iii) The expectation value of operator p^2 (p is momentum operator) is

(a) 0 (b) $\hbar^2\pi^2/32mL^2$ (c) $\hbar^2\pi^2/16L^2$ (d) $\hbar^2\pi^2/8L^2$

10 The quantum mechanical virial theorem for a general potential V(x, y, z)is given by $\left\langle x, \frac{\partial y}{\partial x} + y\frac{\partial v}{\partial y} + z\frac{\partial v}{\partial z} \right\rangle = 2T$, where T is the kinetic energy operator and <> indicates expatiation value, This laeads to the following relation between the expectation value of kinetic energy and potential energy for a quantum mechanical harmonicoscillator problem with potental

$$V = \frac{1}{2}k_x x^2 + \frac{1}{2}K_y y^2 + \frac{1}{2}K_z z^2$$

(a) <T> = <V> (b) <T> = –1/2<V>

(c) <T> = 1/2<V> (d) <T> = – <V>

11. The lowest energy level that is the example of accidental degeneracy, for a particle confined to move in a 3D cubic box of length a is

(a) $12\hbar^2\pi^2/ma^2$ (b) $12\hbar^2\pi^2/8ma^2$

(c) $27\hbar^2\pi^2/ma^2$ (d) $27\hbar^2\pi^2/8ma^2$

12. The degeneracy corresponding to energy of 2D square box with energy $10\pi^2\hbar^2/2ml^2$ is

(a) 2 (b) 3 (c) 4 (d) 5

13. The lowest energy level that exist both in 1 D box and 2 D square box of length l is

(a) $25\hbar^2\pi^2/2ml^2$ (b) $25\hbar^2\pi^2/8ml^2$

(c) $5\hbar^2\pi^2/2ml^2$ (d) $\hbar^2\pi^2/ml^2$

14. The degeneracy of quantum mechanical particle of a cubix box having energy four times that of the ground state energy is

(a) 3 (b) 6 (c) 1 (d) 4

15. A particle is confined in a 3D cubic well of width L with imprentable wall, the degeneracy of 4th level is given by

(a) 1 (b) 2 (c) 3 (d) 4

×××××

QUANTA POINT

DPP- (9) Quantum Chemistry

1. The groud state energy of a particle of mass m in a three dimensional cubic box of side L is not zero but $3h^2/8mL$. This is because

   (a) The groud state has no nodes in the interior of the box

   (b) This is the most convenient choice of the zero level of potential energy

   (c) Position and momentum cannot be exactly determined simultaneously

   (d) The potential at the boundaries is not really infinite, but just very large.

2. A π electron (mass m) in a naphthalene may be modeled as a particle in Two Dimensional box of dimensions a and 2a. The expression for allowed energy level of particle are {n1 and n2 are quantum number that take values 1, 2, 3, ...}

   (a) $\left\{h^2\pi^2/2m\right\}\left\{\left(n_1^2/a^2\right)+\left(n_2^2/a^2\right)\right\}$

   (b) $\left\{\hbar^2\pi^2/2m\right\}\left\{\left(n_1^2/a^2\right)+\left(4n_2^2/a^2\right)\right\}$

   (c) $\left\{\hbar^2\pi^2/2m\right\}\left\{\left(n_1^2/a^2\right)+\left(2n_2^2/a^2\right)\right\}$

   (d) $\left\{\hbar^2\pi^2/2m\right\}\left\{\left(n_1^2/a^2\right)+\left(n_2^2/4a^2\right)\right\}$

3. The degengeracy of an excited state of a particle in a 3-dimensional cubic box with energy 3 times it's ground state energy is

   (a) 3 (b) 2 (c) 1 (d) 4

4. Consider a two-dimensional harmonic oscillator with potential energy $V(x,y)=\frac{1}{2}k_x x^2+\frac{1}{2}k_y y^2$. If $\psi_{nx}(x)$ and $\psi_{ny}(y)$ are the eigen functions and E_{nx} and E_{ny} are the eigenvalues of harmonic oscillator problem in x and y direction with potential $\frac{1}{2}k_x x^2$ and $\frac{1}{2}k_y y^2$ respectively, the wave function and eigen values of the above two dimensional harmonic oscillator problem are

   (a) $\psi_{nx,ny}=\psi_{nx}(x)+\psi_{ny}(y)$
   $E_{nx,ny}=E_{nx}+E_{ny}$

   (b) $\psi_{nx,ny}=\psi_{nx}(x)\,\psi_{ny}(y)$
   $E_{nx,ny}=E_{nx}+E_{ny}$

   (c) $\psi_{nx,ny}=\psi_{nx}(x)+\psi_{ny}(y)$
   $E_{nx,ny}=E_{nx}E_{ny}$

   (d) $\psi_{nx,ny}=\psi_{nx}(x)\psi_{ny}(y)$
   $E_{nx,ny}=E_{nx}\,E_{ny}$

5. A two dimensional square rigid box of side L contains six non interacting electron at T= 0 K. The mass of electron is m. The ground state energy of the system of electron in unit $\pi^2\hbar^2/mL^2$

QUANTA POINT

(a) 8 (b) 10 (c) 12 (d) 16

6. A particle is confined in a 3D cubic well of width L with imprentable wall (i) the sum of the energy of third and fourth energy level is

(a) $10\pi^2\hbar^2/mL^2$ (b) $10\pi^2\hbar^2/3mL^2$ (c) $11\pi^2\hbar^2/2mL^2$ (d) $15\pi^2\hbar^2/2mL^2$

7. A particle of mass m is confined in a two dimensional square well potential of dimension (a). This potential is given by V = 0 for $0 < x < a$ and $0 < y < a$, V = infinite elsewhere. The energy of the first excited state is

(a) $\pi^2\hbar^2/ma^2$ (b) $2\pi^2\hbar^2/ma^2$ (c) $5\pi^2\hbar^2/2ma^2$ (d) $4\pi^2\hbar^2/2ma^2$

8. Compare the difference of energies of the first excited and ground states of a particle confined in (i) a 1-d box (Δ_1), (ii) a 2-d square box (Δ_2) and (iii) a 3-d cubic box (Δ_3). Assume the length of each of the boxes is the same. The correct relation between the energy differences $\Delta_1, \Delta_2, \Delta_3$ for the three cases is

(a) $\Delta_1 > \Delta_2 > \Delta_3$ (b) $\Delta_1 = \Delta_2 = \Delta_3$ (c) $\Delta_3 > \Delta_2 > \Delta_1$ (d) $\Delta_3 > \Delta_1 > \Delta_2$

9. The ratio of energy of first excited state to the ground state of a particle in 3D box of length L and L/2 is

(a) 3 : 2 (b) 2 : 1 (c) 4 : 1 (d) 4 : 3

10. The lowest quantum mechanical energy of particle confined in 1D box of size L is 2 eV. `The energy of quantum mechanical ground state for a system of three non interactive spin 1/2 particle is

(a) 6eV (b) 10 eV (c) 12 eV (d) 16 eV

11. The degeneracy of state having energy $(27h^2/8mL^2)$ for a particle in 3D cubic box of length L is

(a) 4 (b) 3 (c) 2 (d) 1

12. Consider a system of eight non interacting, identical quantum mechanical particle of spin 3/2 in a 1D box of length L. the minimum excitation energy of the system in unit of $h^2/8mL^2$ is

(a) 3 (b) 5 (c) 7 (d) 9

13. For a model system of three non-interacting electron confined in two dimensional square box of length L, the ground state energy in units of $(h^2/8ml^2)$is

(a) 14 (b) 6 (c) 4 (d) 9

14. A particle of mass 'm' is confined in a two-dimensional infinite square well potential of side 'a'. The eight energy of the particle in a given state is $25\hbar^2\pi^2/ma^2$. The state is

(a) 4 fold degeneate (b) 3 fold degenerate

(c) 2 fold degenerate (d) Non-degenerate

15. The one electron states for non interacting electron confined in a cubic box of side a are $E_0 < E_1 < E_2 < E_3$ etc

(i) the energy of the lowest state is

(a) 0 (b) $\pi^2\hbar^2/2ma^2$ (c) $\pi^2\hbar^2/ma^2$ (d) $3\pi^2\hbar^2/2ma^2$

QUANTA POINT

DPP- (10) Quantum Chemistry

1. The hydrogenic orbital with the form of the radial function, $r^2(\alpha_1 - r)(\alpha_1 - r)\exp[-\beta r]$ where α_1, α_2 and β Are constants, May be identified as a

   (a) 3d orbital (b) 4f orbital (c) 3d orbital (d) 5f orbital

2. The position of radial node for an electron in 2s orbital of hydrogen atom is {given that $R_{2.0}\alpha\left[\left(2-\{r/a_0\}\right)\right]e^{-r/2a_0}\}$

   (a) $r = 2a_0$ (b) $r = a_0$ (c) $r = a_0/2$ (d) no radial node

3. The normalisation constant corresponding to radial part of wave function $R_{(r)} = e^{-ra_0}$ is

   (a) $2\,a_0^{3/2}$ (b) $2\,a_0^{-3/2}$ (c) $2\,a_0^{1/2}$ (d) $2\,a_0^{-1/2}$

4. A hydrogenic 3 p orbital has the following form of the radial wave function (α_i = constant)

   (a) $r(\alpha_1 - r)e^{-\alpha 2r}$ (b) $r^2e^{-\alpha 3r}$ (c) $r^2(\alpha_4 - r)(a_5 - r)e^{-\alpha 6r}$ (d) $r^3e^{-\alpha 7r}$

5. A hydrogenic orbital with radial function of the form $r^\alpha \exp[-\beta r]$ and ϕ - part as $\exp[-3i\,\phi]$ corresponds to

   (a) $n > 4, l > 3, m = 3$ (b) $n > 4, l = 3, m = -3$

   (c) $n > 4, l = 3, m = 3$ (d) $n = 4, l = 3, m = -3$

6. The radial part of wave function $R_{2,1}$ is maximum at

   (a) $r = a_0$ (b) $r = 2a_0$ (c) $r = 0$ (d) r = infinite

7. The orbital with two radial and two angular nodes is

   (a) 3p (b) 5d (c) 5f (d) 8d

8. An atomic state of hydrogen atom is represented as $\psi = \left(1/2a_0^3\right)^{0.5} r\left[1-\left(r/2a_0\right)\right]e^{-r/3a_0}\cos\theta$, where a_0 is constant value. The quantum number of the state are

   (a) $l = 0, m = 0, n = 1$ (b) $l = 1, m = 1, n = 2$

   (c) $l = 1, m = 0, n = 3$ (d) $l = 1, m = 1, n = 3$

9. The radial part of a hydrogenic wave function is given by $r(\alpha - r)e^{-\beta r}$ (α and β are constant). This function is then identified as

QUANTA POINT

(a) 2s (b) 3p (c) 4d (d) 5f

10. $\psi = Nr(6-Zr)e(-Zr/3)\cos\theta$ is a proposed hydrogenic wavefunction, where Z = atomic number, r = radical distance from the nucleus, θ = azimuthal angle N is constant. The incorrect statement above ψ is

(a) $\psi = 0$ in the xy plane

(b) two radical nodes are present in ψ

(c) one angular node is present in ψ

(d) the size of orbital decreases with increase in atomic number

11. The un-normalized radial wave function of a certain hydrogen atom eigenstate is $(6r-r^2)e^{-r/3}$. A possible angular part of the eigen state is

(a) $5\cos^3\theta - 3\cos$ (b) $3\cos^2\theta - 1$ (c) $\cos\theta$ (d) 1

12. An unnormalized wavefunction of the hydrogen atom is given by $r^2 e^{-r/3}(3\cos^2\theta - 1)$, the three quantum number n, l, m associated with this orbital respectively are

(a) 2, 2, 0 (b) 2, 1, 1 (c) 3, 2, 0 (d) 3, 1, 1

13. Hydrogenic atomic orbital is given by $N r^2 e^{-r/3a0}(3\cos^2\theta - 1)$ represents

(a) 2p orbital (b) 3p orbital (c) 3 d orbital (d) 4d orbital

14. The angular part of the wave function for the electron in a hydrogen atom is proportional to $\sin^2\theta\cos\theta e^{2i\theta}$. The value of the azimuthal quantum number l and the magnetic quantum number (m) are respectively.

(a) 2 and 2 (b) 2 and -2 (c) 3 and 2 (d) 3 and -2

15. Which of the following is true for the radial part of the hydrogen and wave function $R_{n,l}(r)$ (n) principal quantum number and the nodes associated with them?

(a) The radial part of only s function is non-zero at the origin and has (n – 1) nodes
(b) The radial part of s function is zero at the origin and has n number of nodes
(c) All radial functions have values of zero at the origin and have (n – 1) nodes
(d) The radial parts of all s functions are zero at the origin and have no nodes.

QUANTA POINT

DPP- (11) Quantum Chemistry

1. The energy of 2s and 2p orbitals is the same for

(a) Li (b) Li^{2+} (c) Be^{2+} (d) H^{+}

2. If the ionization energy of H atom is x, the ionizaton energy of Li^{2+}, is

(a) 2x (b) 3x (c) 9x (d) 27x

3. The spherical harmonics function $Yl,m(\theta,\Phi)$, with appropriate value of *l* and m, is an eigen function of $Lx^2 + Ly^2$ operator. The corresponding eigenvalue is

(a) $\left(l(l+1)-m^2\right)\hbar^2$ (b) $\left(l(l+1)+m^2\right)\hbar^2$

(c) $l(l+1)\hbar^2$ (d) $m^2\hbar^2$

4. Consider the statements

(i) the radial part of wave function of S orbital of hydrogenic atom is non-zero at origin because radial part is containing of r^1 terms.

(ii) The degeneracy corresponding to energy value $-e^2/72\pi\varepsilon_0 a_0$ for an electron in an orbital of hydrogen atom is 9

(iii) If angular part is contianing of only $\cos\Theta$ term than the value of $l = 0$

The correct statements above are

(a) (i), (ii) (b) (ii), (iii) (c) (i), (iii) (d) all

5. The orbital degenracy of the level of a one-electron atomic system with Z = 5 and energy –3.4eV, is

(a) 1 (b) 5 (c) 25 (d) None

6. For H-like atoms the group state energy is proportional to

(a) $\frac{\mu}{Z^2}$ (b) $\frac{Z^2}{\mu}$ (c) μZ^2 (d) $\frac{1}{\mu Z^2}$

7. An electron is found in an orbital with one radical node and two angular node. Which orbital the electrons is in ?

(a) 1s (b) 2s (c) 3d (d) 4d

8. The expectation value of p^2 of a particle in a cubic box of side *l*, having the

wavefunction $\Psi_{n_x,n_y,n_z}(x,y,z) = \left(\frac{2}{l}\right)^{3/2} \sin\frac{2\pi x}{l}\sin\frac{3\pi y}{l}\sin\frac{2\pi z}{l}$, is/are

QUANTA POINT

(a) $\frac{17h^2}{4l^2}$ (b) $\frac{7h^2}{4l^2}$ (c) $\frac{3h^2}{l^2}$ (d) $\frac{13h^2}{4l^2}$

9. For an electron in 1s orbital of He^+, the average value of r, <r> is

(a) $\frac{3}{2}a_0$ (b) $\frac{3}{4}a_0$ (c) $3a_0$ (d) $\frac{1}{2}a_0$

10. The degeneracy of the energy level with n = 6 (n being the principal quantum number) in a hydrogenic atom or ion?

(a) 16 (b) 9 (c) 36 (d) 25

11. In an hydrogen atom the coulomb degeneracy for the n = 4 state is

(a) 4 (b) 16 (c) 18 (d) 32

12. An electron in the Li^{2+} atom is in a state whose energy is –3.4 eV the degeneracy of the state is

(a) 4 (b) 16 (c) 36 (d) None

13. The energy of a hydrogen atom in a state is $-\left[R_H hc/25\right]$ (R_H = Rydberg constant). The degeneracy of the state is

(a) 5 (b) 10 (c) 25 (d) 50

14. The orbital degeneracyof the level of a one electron atomic system with z = 5 and energy $\approx -13.6\ eV$, is

(a) 1 (b) 5 (c) 25 (d) 36

15. A particle is in state $\Phi = \psi_1 + 3\psi_2$, where ψ_1 and ψ_2 are eigenfunctions of the Hamiltonian of the particle with eigenvalues E_1 and E_2, respectively. The average energy of the particle in the state Φ is

(a) $(E_1 + 9E_2)/10$ (b) $(E_1 + 3E_2)$

(c) $(E_1 + 9E_2)/4$ (d) $(E_1 + 3E_2)/10$

×××××

QUANTA POINT

DPP- (12) Quantum Chemistry

1. The correct normalized wavefunction for one of the sp^2 hybrid orbital is

(a) $\frac{1}{3}\psi_{2s}+\frac{1}{3}\psi_{2p_x}+\frac{1}{3}\psi_{2p_y}$ (b) $\frac{1}{\sqrt{3}}\psi_{2s}+\frac{2}{\sqrt{3}}\psi_{2p_x}+\frac{1}{\sqrt{6}}\psi_{2p_y}$

(c) $\frac{1}{\sqrt{3}}\psi_{2s}+\frac{1}{\sqrt{2}}\psi_{2p_x}+\frac{1}{\sqrt{6}}\psi_{2p_y}$ (d) $\frac{1}{\sqrt{3}}\psi_{2s}+\frac{1}{2\sqrt{3}}\psi_{2p_x}+\frac{1}{\sqrt{6}}\psi_{2p_y}$

2. The function of a certain system is linear combination $\psi=\sqrt{\frac{1}{4}}\psi_1+\sqrt{\frac{3}{4}}\psi_2$ where ψ_1 and ψ_2 are energy eigen functions with eigen values (non-degenerate) E_1 and E_2, respectively. What is the probability that the system energy will be observed to be E_1?

(a) $\sqrt{\frac{3}{16}}$ (b) $\frac{3}{4}$ (c) $\frac{1}{4}$ (d) $\sqrt{\frac{1}{4}}$

3. A doubly ionized lithium atom in an excited state (n = 6) emits a photon of energy 4.25eV. What are the quantum number (n) and the energy (E) of the final state?

(a) n = 2, E = – 30.6 eV (b) n = 3, E = –13.6 eV

(c) n = 4, E = –7.65 eV (d) n = 5, E = –4.90 eV

4. The angular momentum operator Lz has eigen functions of the form $\exp i A\Phi$. The condition that a full rotation leaves such as an eigen function unchanged is satisfies for all the values of A.

(a) $0,\pm\frac{1}{3},\pm\frac{2}{3},\pm1,\pm\frac{4}{3}\ldots$ (b) $0,\pm1,\pm2,\pm3\ldots$ (c) $0,\pm\frac{1}{2},\pm1,\pm\frac{3}{2}\ldots$ (d) $0,\pm\frac{1}{2},\pm\frac{3}{2},\pm\frac{5}{2}\ldots$

5. For a particle in a 1-D box of length 2L the normalizaton constant A for its wavefunction $\psi(x,t)=A\sin\left(\frac{n\pi x}{2L}\right)$ (where n = 1, 2,3 ....) is given by

(a) $A=\sqrt{\frac{1}{L}}$ (Key; the length is 3L sp replace L with 2L in the standard answer C or explict normalization

(b) $A=\sqrt{\frac{1}{2L}}$

(c) $A=\sqrt{\frac{2}{L}}$

QUANTA POINT

(d) $A = \sqrt{\frac{1}{4L}}$

6. Which of the following set(s) of quantum numbers is are NOT allowed?

(a) n = 3, 1 = 2, ml = –1 (b) n = 4, l = 0, ml = –1

(c) n = 3, l = 2, ml = –3 (d) n = 5, l = 3, ml = –2

7. Consider a one-dimensional infinite potential well of width a. The system contains five non-interacting electrons, each of mass m, at temperature T = 0L. The energy of the highest occupied state is

(a) $\frac{25\pi^2h^2}{2ma^2}$ (b) $\frac{10\pi^2h^2}{2ma^2}$ (c) $\frac{5\pi^2h^2}{2ma^2}$ (d) $\frac{9\pi^2h^2}{2ma^2}$

8. A particle of mass m is in an infinite square well potential of length L. It is in a superposed state of the first two energy eigenstates, as given by $\psi(x) = \frac{1}{\sqrt{3}}|\psi_{n=1}(x) + \sqrt{\frac{2}{3}}\psi_{n=2}(x)$. Identify the correct statement(s), h is Planck's constant

(a) <P> = 0 (b) $\Delta p = \frac{\sqrt{3h}}{2L}$ (c) $<E> = \frac{3h^2}{8mL^2}$ (d) $\Delta x = 0$

9. The most probable radius corresponding to 1s orbital of hydrogen atom is

(a) 1.5 a_0 (b) a_0 (c) $2a_0$ (d) $3a_0$

10. A particle of mass m is in one dimensional potential $V(x) = \begin{cases} 0 & 0 < x < L \\ \infty, \text{otherwise} \end{cases}$ At some instant its wave function is given by $\psi(x)$ are the ground and the first excited states, respectively. Identify the correct statement

(a) $<x> = \frac{L}{2}; <E> \frac{h^2}{2m}\frac{3\pi^2}{L^2}$ (b) $<x> = \frac{2L}{3}; <E> \frac{h^2}{2m}\frac{\pi^2}{L^2}$

(c) $<x> = \frac{L}{2}; <E> \frac{h^2}{2m}\frac{8\pi^2}{L^2}$ (d) $<x> = \frac{2L}{3}; <E> \frac{h^2}{2m}\frac{4\pi^2}{3L^2}$

11. One to the correct normalized sp^2 hybrid orbitals is

(a) $\frac{1}{3}\Phi_{2s} + \frac{1}{3}\Phi_{2p_x} + \frac{1}{3}\Phi_{2p_y}$

(b) $\frac{1}{2}\Phi_{2s} + \frac{\sqrt{3}}{\sqrt{8}}\Phi_{2p_x} + \frac{\sqrt{3}}{\sqrt{8}}\Phi_{2p_y}$

(c) $\frac{1}{\sqrt{3}}\Phi_{2x} + \frac{\sqrt{2}}{\sqrt{3}}\Phi_{2p_x}$

(d) $\frac{1}{3}\Phi_{2y} + \frac{2}{3}\Phi_{2p_x}$

12. Suppose the wave function of a one dimensional system is $\psi = \sin(kx)\exp(3ikx)$, the value of momentum is

(a) 0 (b) $\hbar k$ (c) $2\hbar k$ (d) $3\hbar k$

QUANTA POINT

13. The correct statement about the symmetry of the eigenfunction of a quantum of 1-D harmonic oscillator is

(a) All the eigen functions are only even functions, because the potential is an even function

(b) All the eigen functions are only odd functions, although the potential is an even function

(c) The eigen functions have no odd-even symmetry

(d) All the eigen function are either odd or even functions, because the potential is an even function

14. Consider a model system of five non-interacting ferminons in a single 3-dimensional oscillator. The Hamiltonian of single particle is $\hat{H}=\frac{1}{2m}\left(\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2\right)+\frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right)$; where m is the mass of the particle, ω is the angular frequency, $\hat{p}_x, \hat{p}_y$ and $\hat{p}_z$ are the momentum operators.The ground state energy of the system of 5 non-interacting ferminons is

(a) $\frac{21}{2}\hbar\omega$ (b) $\frac{15}{2}\hbar\omega$ (c) $\frac{5}{2}\hbar\omega$ (d) $\frac{25}{2}\hbar\omega$

15. Consider a classical harmonic oscillator with a mass m and a force constant k oscillating with a freqeuncy v. Which of the following statements is NOT true for this system?

(a) v increases if m decreases

(b) The oscillator is most likely to be found at its equilibrium position

(c) The acceleration is maximum at its turning points

(d) v does not depend on how large the amplitude of the oscillation is

×××××

QUANTA POINT

DPP- (13) Quantum Chemistry

1. The quantum mechanical virial therorem of a general potential V (x,y,z) is given by $\langle x(\partial V/\partial x)+(\partial V/\partial y)+z(\partial V/\partial z)\rangle = 2T$, where T is the kinetic energy operator and indicates expa tiation value. This leads to the following relation between the expectation value of kinetic energy and potential energy for a quantum mechanical harmonic oscillator with potential

$$V=\left(\frac{1}{2}\right)K_xX^2+\left(\frac{1}{2}\right)K_yY^2+\left(\frac{1}{2}\right)K_zZ^2$$

(a) $<T>=<V>$ (b) $<T>=-1/2<V>$

(c) $\langle T\rangle=\frac{1}{2}\langle V\rangle$ (d) $\langle T\rangle=-\langle V\rangle$

2. The correct statement about HCl and DCl, among the following, is

(a) DCl has a smaller zero-ponit energy than HCl

(b) HCl has a smaller vibration frequency than DCl

(c) The force constant k of the HCl bond is half that of DCl

(d) The reduced mass of DCl is smaller that that of HCl

3. Consider the statement

(i) Function ψ_o and ψ_1 are orthogonal to each othe in 1-D SHO.

(ii) The average value of kinetic energy in first excited state in case of 1-D SHO is 0.75 hv.

(iii) Maxumum amplitude in SHO is a classical term that may be obtained by equating potential energy to the kinetic energy. The correct statements above are

(a) (i), (ii) (b) (ii) ,(iii) (c) (i) , (iii) (d) (i), (ii) , (iii)

4. Consider the statements

(i) At very high value of quantum number two large maximum at the extremum of vibration in Simple Har monic Oscillatro,

(ii) The wavefunction of harmonic oscillator ither symmetric or antisymmetric under reflection through x= 0.

(iii) SHO model is an ideal situation inrelity the bibrations that takes place is anharmonic in nature.

(iv) Thermal decomposiiton of molecule may be explained by SHO.

The true statements above are

(a) (i),(ii),(iii) (b) (ii),(iii),(iv) (c) (i),(iii),(iv) (d) All

5. The mathematical expressions $e^{-i(kx-wt)}$ represents

(a) A wave stationary in space but oscillating in time

(b) A travelling wave moving in the positive x-direction

QUANTA POINT

(c) A wave stationary in time but peridiocally varying in space

(d) A travelling wave moving in the negative x-direction

6. For a particle undergoing quantum tunneling through a barrier, which of the following is NOT true

(a) The amplitude the particle wave function after passing the barrier decreases with an increase in tunneling distance

(b) The probability of finding the particle after passing the barrier decreases with increase in tunneling barrier height

(c) The energy of the particle after crossing the barrier decreases with increase in tunneling distance

(d) The change in the phase of the particle wave function upon transmission is proportional to the tunneling distance

7. The position of a particle in space has a Gaussian probability distribution function. This implies the underlying potential energy surface for the particle

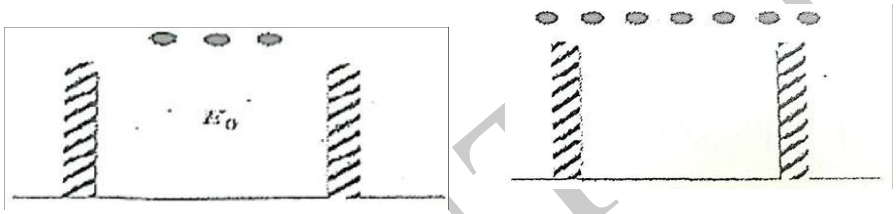
(a) Is flat in space

(b) has a linear dependencce on spatial coordinate

(c) has a quadratic dependent on spatial coordinate

(d) has a cubic depenedence on spatial coordinate

8. A quantum mechanical system consist of 1-D infinite box, as indicated in the figure below



state energy of the system is found to be E_0 = 18 eV. If 7(seven) such identical particles are placed in the box then the ground state energy, in units of eV is

(a) 66 eV (b) 33 eV (c) 132 eV (d) 264 eV

9. The number of degenerate spatial orbitals of a hydrogen-like atom with principal quantum number n = 6

(a) 12 (b) 6 (c) 72 (d) 36

10. When a particle with mass m energy E higher than potential barrier V strikes the batrier with infinite width ther expression of transmission coefficient is

(a) $T = e^{\sqrt{2m(V-E).L/\hbar}}$ (b) $T = \sqrt{2m(V-E).L/\hbar}$ (c) $T = e^{-2\sqrt{2m(V-E).L/\hbar}}$ (d) $T = \left\{\frac{4P_1P_2}{(P_1+P_2)}\right\}$

11. If mass of the particle becomes fourth times then the decay length in case of tunneling becomes

(a) Half (b) Two times (c) 1/4 (d) fourth times

12. Consider the statement

(i) If a particle with energy E move and collides with a potential barrier of height V (V < E) and infinite width then the movement of particle in 1 region in +x direction is e^{ikx}.

(ii) If a particle with energy E move and collides with a potential barrier of height V (V = E) and infinite width then

the transmission coefficient is not zero.

(iii) If a particle with energy E move and collides with a potential barrier of height V (V > E) and finite width then the reflection coefficient increases with mass.

The true statements above are

(a) (i), (ii) (b) (ii), (iii) (c) (i), (ii), (iii) (d) (i) only

13. The probability current density in potential barrier problem is

(a) $J = (h/4\pi im)\{\psi^*\delta(\psi\delta/x)\} - \psi(\delta\psi^*/\delta x)$

(b) $J = -(h/4\pi im)\{\psi^*\delta(\psi\delta/x)\} - \psi(\delta\psi^*/\delta x)$

(c) $J = (h/2\pi im)\{\psi^*\delta(\psi\delta/x)\} - \psi(\delta\psi^*/\delta x)$

(d) $J = -(h/2\pi im)\{\psi^*\delta(\psi\delta/x)\} - \psi(\delta\psi^*/\delta x)$

14. Consider the statement

(i) Tunneling provides another mechanism to convert reactants to products that does not require an increase in energy of the reactants for the reaction to proceed.

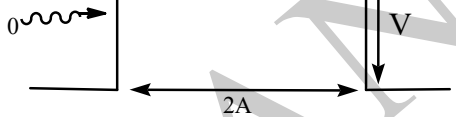
(ii) heavier atom tunneling is only appreciable if (V – E) is very small

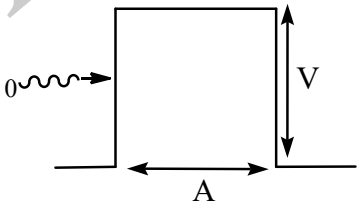
(iii) Quantum mechanical particle can escape through the barrier even through it does not have sufficient energ to go over the barrier

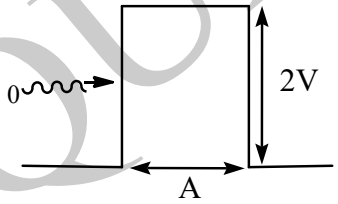
The true statement above are

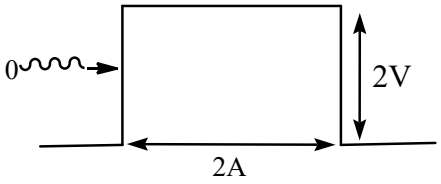
(a) (i),(ii) (b) (ii),(iii) (c) (i), (iii) (d) All

15. A quantum particle with fixed initial energy $E_0 < V$ is allowed to strike the following four barriers separately. The transmission probability is maximum in

(a)


(b)


(c)


(d)


QUANTA POINT

DPP- (14) Quantum Chemistry

1. Consider the statements
(1) First order correction to the ground state energy is the expectation value corresponding to perturbed part of Hamiltonian when we take perturbed part of function into consideration.
(2) When the value of first order energy correction because of perturbation becomes zero then we apply second order or higher order perturbation.
(3) Perturbation method generally apply when the deviation of the real system from ideality is large.
Correct statements above are
(a) (1),(2) (b) (2),(3) (c) (1),(2), (3) (d) (2) only

2. The quantum state of a particel moving in a circular pathin plane is given $b\psi = (2\pi) - 1/2e^{-im\phi}$ for rotating particle in m state) when a perturbation $H_{1=P\cos}\ \varphi$ is applied (P is constant), what will be the first order correction to the energy of the m^{th} state is
(a) 0 (b) $P/2\pi$ (c) $P/4\pi$ (d) $Pm^2/4\pi^2$

3. First order perturbation correction ΔE_n^1 to the energy level E_n of simple h armonic oscillator due to anharmonicity perturbation is given by
(a) $\Delta E_n^1 = \gamma$ (b) $\Delta E_n^1 = \gamma^2$ (c) $\Delta E_n^1 = \gamma^{-1}$ (d) $\Delta E_n^1 = 0$

4. A particle in a one dimensional harmonic oscillator in x-direction is perturbed by a potential λx (λ is a num ber). The first order correction to the energy of the ground state
(a) is zero (b) is negative
(c) is positive (d) may be negative or positive but NOT zero

5. An oscillator is governed by the potential $V = (k/2)x^2 + (\gamma/6)x^3 (b/24)x^4$ using a harmonic oscillator as an unperturbed problem, calculate the first order correction to the energy of the ground state in simple harmonic oscillator is
(a) $b/32\gamma\beta^2$ (b) $b/32\beta$ (c) $\gamma b/32\beta^2$ (d) $b/32\beta^2$

6. When we operate perturbed part of Hamiltoman H = P sin Φ on rotating particle. Then first correction to the energy is Wavefunction is $\psi_m(\Phi) - \left\{1/\sqrt{2\pi}\ e^{im\Phi}\right\}$
(a) P (b) $P/2\pi$ (c) $P2/4\pi2$ (d) 0

7. Particle is confined to move in a 1D box of length –L to –L, the system is perturbed by b(a–x) then first order correction to the ground state energy is
(a) ba/2 (b) ba (c) ba/4 (d) 2ba

8. A particle is confined to move in 1D box of length 2a($-a < x < a$) with V = 0 inside and infinite else where
(i) The function corresponding to first excited state is

(a) $(1/a)^2 \cos(\pi x/a)$ (b) $(1/a)^2 \sin(\pi x/a)$

(c) $(2/a)^{1/2} \cos(2\pi x/a)$ (d) $(2/a)^{1/2} \sin(2\pi x/a)$

9. If the system is perturbed by $V = \delta\{x - (a/2)\}$ then first order energy correction to first excited state is

(a) 0 (b) 2/a (c)1/a (d)1/2a

10. A particle is confined to move in 1D box of length L, if system is perturbed by $\delta\{x - (L/2)\}$. Then first order energy correction to the ground state

(a)2/L (b) L/2 (c)1/L (d) 0

11. Consider a particle in a one dimensional box of length 'a' with the following potential

$V(x)\infty = x < 0$

$V(x)\infty = x > 0 V(x) = 0; 0 \le x \le a/2, V(x) = V a/2 \le x \le a$

Starting with the standard particle in a box Hamiltonian as the Zeorth order Hamiltonian and the potential of V_1 from 'a/2' to 'a' as a perturbation, the first order energy correction to the ground state is

(a) V_1 (b) $V_1/4$ (c) $-V_1$ (d) $V_1/2$

12. A particle is confined to move in a 1D box of length L, the left half of the box is perturbed by V_1 and right half ot the box is perturbed by $V_1/2$, First order correction to the ground energy because of perturbation is

(a) $\frac{V_1}{4}$ (b) $\frac{3V_1}{4}$ (c) $\frac{5V_1}{4}$ (d) $\frac{3V_1}{2}$

13. A one-dimensional anharmonic oscillator is treated by perturbation theory. The harmonic oscillator is used as the unperturbed system and the perturbation is $\left[\left(\frac{1}{6}\right)\gamma x^3\right]$ (γ is a constant) Using only the first order correction, the total ground state energy of anharmonic oscillator is

(Note : For a one-dimensional harmonic oscillator $\psi_0(x) = [\alpha/\pi]^{1/4} e^{-\alpha x^2}$

(a) $\frac{1}{2}\hbar\left(\frac{k}{\mu}\right)^{1/2}$ (b) $\left(\frac{1}{2}+\frac{\gamma}{6}\right)\hbar\left(\frac{k}{\mu}\right)^{1/2}$ (c) $\left(\frac{1}{2}+\frac{\gamma}{3}\right)\hbar\left(\frac{k}{\mu}\right)^{1/2}$ (d) $\left(\frac{1}{2}+\frac{\gamma}{12}\right)\hbar\left(\frac{k}{\mu}\right)^{1/2}$

14. A one-dimensional quantum harmonic oscillator is perturbed by a potential γx^3. The first order correction to the energy for the ground state ΔE_0^1 is

(a) $\Delta E_0^1 > 0$ but < 1 (b) $\Delta E_0^1 < 0$ (c) $\Delta E_0^1 = 0$ (d) $\Delta E_0^1 > 2$

QUANTA POINT

DPP- (15) Quantum Chemistry

1. A certain 2- level system has stationary state energies E_1 and E_2 ($E_1 < E_2$) and with nornalized wave functions ϕ_1 and φ_2 respectively. In the presence of a perturbation, the second -order correaction to the energy for the first state will be

(a) $\frac{\langle \phi_1 | V | \phi_2 \rangle}{E_1 - E_2}$ (b) $\frac{\langle \phi_2 | V | \phi_1 \rangle}{E_2 - E_1}$ (c) $\frac{\langle \phi_2 | V | \phi_1 \rangle^2}{E_1 - E_2}$ (d) $\frac{\langle \phi_2 | V | \phi_1 \rangle^2}{(E_1 - E_2)^2}$

2. A particle of mass m is confined in potential well given by V (x) = 0 for -L/2 < x < L/2 and V (x) infinite elsewhere. A perturbing potential H'(x) = α x has been applied to the system. Let the first and second order corrections to ground state be $E_0^{(1)}$ and $E_0^{(2)}$ respectively Which one of the following statement is correct

(a) $E_0^{(1)} < 0$ and $E_0^{(2)} > 0$ (b) $E_0^{(1)} = 0$ and $E_0^{(2)} > 0$

(c) $E_0^{(1)} > 0$ and $E_0^{(2)} < 0$ (d) $E_0^{(1)} = 0$ and $E_0^{(2)} < 0$

3. For non-degenerate perturbation theroy for ground state, with $E_0^{(0)}$ as zeroth order cnergy, $E_0^{(1)}$ as the first-order perturbation correction and E_0 as the exact enrgy, which of the following is true ?

(a) $\left(E_0^{(0)} + E_0^{(1)}\right)$ is always equal to E_0 (b) $\left(E_0^{(0)} + E_0^{(1)}\right) \le E_0$

(c) $\left(E_0^{(0)} + E_0^{(1)} \ge E_0\right)$ (d) $E_0^{(0)} \le E_0 \le E_0^{(1)}$

4. The following are the three statements about perturbation theory

(a) Second order perturbation correction to their ground state energy is ALWAYS negative.

(b) Sum of the zeroth order and the first order corrections to the ground state energy is greater than the exact ground state energy

(c) Sum of the zeroth order and firstorder correction to the ground state energy is less than the exact state energy.

From the following which one is correct?

(a) Only (a) is truue (b) Both (a) and (b) are true

(c) Only (c) is true (d) Both (b) and (c) are true

5. An unperturbed 2 level system has energy eign value E_1 and E_2 and has energy eignfunction $\begin{bmatrix}1\\0\end{bmatrix}$ and $\begin{bmatrix}0\\1\end{bmatrix}$ when perturbed its Hamiltonian is represented by $\begin{matrix}E_1 & A\\ A^* & E_2\end{matrix}$

QUANTA POINT

(i) The first order correction to Ei is

(a) 4A (b) 2A (c) A (d) 0

(ii) The second order corrrection to energy E_1 is

(a) 0 (b) A (c) A^2/E_1-E_2 (d) A^{*2}/E_1-E_2

(iii) The first order correction to the wavefunction is

(a) $\begin{bmatrix} 0 \\ A^*/E_1-E_2 \end{bmatrix}$ (b) $\begin{bmatrix} A^*/E_1-E_2 \\ 0 \end{bmatrix}$ (c) $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ (d) $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$

6. For a particle in square box of length L with origin x = 0 and y = 0 if the system is perturbed by H = b for 0.25 L $\leq$ x < 0.75 L $\leq$ x < 0.75L 0.25 L < y < 0.75 L then the first order energy correetion to the ground state is

(a) $\left[1+(2/\pi)\right]b$ (b) $\left[1+(2/\pi)\right]^2 b/4$

(c) $\left[1+(2/\pi)\right]^2 b^2/16$ (d) $\left[1+(2/\pi)\right](b/4)^2$

7. An eign state of energy satisfies $H\psi_n = E_n\psi_n$. In the presence of extra constant potential V_0V

(a) Both En and ψ_n will change (b) Only ψ_n will change but not En

(c) Only En will change not ψ_n (d) Neither En nor ψ_n will change

8. The ground state of a certain system with energy is E_0subjected to a perturbation ΔH yielding first - order correction E_1^0. If is the true ground -state energy of the perturbed system, the inequality that always holds is

(a) $\in_1 \geq 0$ (b) $\in_0 \geq E_0$

(c) $\in_0 + \in_1 \leq E_0$ (d) $\in_0 + \in_1 \geq 0$

9. Which of the following statements on ground state-perturbation theory, involving zero order energy $E_0^{(0)}$, first order energy correction $E_0^{(1)}$ and second order energy correction $E_0^{(2)}$ is false

(a) $E_0^{(1)}$ is the average value of perturbation (operator with respect to ground state of zero order Hamiltonian)

(b) $E_0^{(1)}$ is necessartly negative

(c) $E_0^{(2)}$ is necessarily negative

(d) $E_0^{(0)} + E_0^{(1)}$ is an upper bound to their exact ground state energy

10. The position of a particle in space Gaussian probability distribution function. This implies that the under lying potential energy surface for the particle

(a) 1s flat in spacè

(b) Has a linear dependence on spatial coordinates

(c) Has a quadrafic dependence on spatial coordinates

(d) Has a cubic dependence on spatial coordinates

11. The first-order correction to energy for the ground state of a particle in a box of length L due to a perturbation λx would be

(a) $\lambda L/2$ (b) λL (c) $2/\lambda$ (d) 2

QUANTA POINT

12. The unperturbed energy levels of a system $\in = 0, = 2$ and $\in_2 = 4$. The second order correction to energy for the ground state in presence of the perturbation V for which V 10 = 2. $V_{20} = 4$ and V_{12}=6 has been found to be

(a) –6 (b) 0 (c) +6 (d) –8

13. Consider a particle on ring is perturbed by interacting with an applied electric field (E) with the perturbation being H= μECosΦ , where μ is dipole moment. The energy level correct upto first order are

(a) $\left[m_l^2\hbar^2 / 2I\right] - \left[\mu E / \pi\right]$ (b) $\left[m_l^2\hbar^2 / 2I\right] - \left[\mu E / 2\pi\right]$

(c) $\left[m_l^2\hbar^2 / 2I\right] + \left[\mu E / 2\pi\right]$ (d) $\left[m_l^2\hbar^2 / 2I\right]$

14. The normalized wavefunction of a particel in one dimensional potential well

$$V(x) = \begin{cases} 0 \text{ if } 0 \le x \le a \\ \infty \text{ otherwise} \end{cases}$$

are given by

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi / x}{a}\right), \text{ where } n = 1,2,3,.....$$

The particlei s subjected to a perturbation

$$V'(x) = V_1 \cos\left(\frac{\pi A}{a}\right) \text{for} 0 \le x \le \frac{a}{2}$$

= 0 otherwise

The shift in the ground state energy due to the perturbation, in the first order perturbation theory, is

(a) $\frac{2V_0}{3\pi}$ (b) $\frac{V_0}{3\pi}$ (c) $-\frac{V_0}{3\pi}$ (d) $-\frac{2V_0}{3\pi}$

15. A Particale is confuned as to a one dimensional potental box with the potential V = 00<x<a V = infinite Elsewhere. If the particle is subjected to a perturbation, within the box, W β x, where β is small constant, the first order correction to the ground state energy is

(a) 0 (b) aβ / 4 (c) aβ / 2 (d) aβ

QUANTA POINT

DPP- (16) Quantum Chemistry

1. In a variational method, four classes of trial functions have been applied and the total energy computed. The exact value of the energy is equal to –50.2 eV. Choose the best approximation to this value obtained in correct calculations:
(a) –48.2 eV (b) –50.5 eV (c) –45.3 eV (d) 43.0 eV

2. A trial wave function for SHO was proposed i,e,, $y = (x^2-1)e\text{-}x2$ if the energy calculated by this function is E than which of the below is correct
(a) $E > 0.5\hbar\omega$ (b) $E > 2.5\hbar\omega$ (c) $E > 3.5\hbar\omega$ (d) $E > 4.5\hbar\omega$

3. A trail wavefunction used in SHO e^{-cx^2} was used and energy value was obtained as $\left(\hbar^2 C/2m\right)+\left(m\omega^2/8C\right)$ The minimum value of energy that was obtained by variational principle is
(a) $\frac{\hbar\omega}{2}$ (b) $\hbar\omega$ (c) $\frac{\hbar\omega}{4}$ (d) $2\hbar\omega$

4. The energy calculated for a multielectron atom using variational function is $E=\left(\frac{\alpha\hbar^2}{m}\right)-\alpha^2\hbar$ The value of variational parameter α is
(a) $\frac{\hbar}{m}$ (b) $\frac{\hbar}{2m}$ (c) $\frac{2\hbar}{m}$ (d) None

5. For a particle in box problem in (0,L) an approximate wavefunctionx (5L-x)(L-x). The average energy E for this state is
(a) $\left(\frac{h^2}{8mL^2}\right) < E < \left(\frac{h^2}{2mL^2}\right)$ (b) $E > \left(\frac{h^2}{2mL^2}\right)$
(c) $\left(\frac{h^2}{4mL^2}\right) < E < \left(\frac{h^2}{2mL^2}\right)$ (d) $0 < E < \left(\frac{h^2}{8mL^2}\right)$

6. Consider the statements
(i) A trial wavefunction $(2\text{-}r)e^{-ar}$ is suitable for an electron in 2p orbital
(ii) The expectation value of the energy calculated with any function *f*Ö obeying the same boundary conditions as the correct system wave functions cannot be lower than Egs.
(iii) Trial wave function with more than one parameter can produce impressive result but price we have to pay for that is lengthly calculation.
Correct statements are above are
(a) (i), (ii), (iii) (b) (ii), (iii) (c) (i), (ii) (d) (i), (iii)

QUANTA POINT

7. Consider the statement
(i) Variational principle is valid for ground sate only
(ii) If the variatonal function is orthogonal to exact solutions to the Schrodfnger equation that correspond to all the states of lower energy than the state we are interested in the variational principle is still valid.
(iii) Variational method Φ stands for the trial function, H the Hamilton, E_0 the exact ground state energy, and ψ_0 the exact ground -state function , $\varepsilon = \langle \Phi\Phi \rangle / \langle \Phi\Phi \rangle$, If $\varepsilon = E_0$ this means that : $\psi_0 = E_0$ The correct statements is /are
(a) (i), (ii) (b) (ii) (c) (i), (ii), (iii) (d) (i), (iii)

8. Consider the statement
(i) A trial wavefunction that depends linearly on variational parameter, leads to secular determinant.
(ii) We choose the smallest root of secular determinant in calculating, the ground state from variational principle
(iii) Perturbation theory express the solution to one problem in another problem solves previously The correct statements above is/are
(a) (i),(ii) (b) (ii),(iii) (c) (i),(iii) (d) (i),(ii),(iii)

9. For some one electron system with I = 0 and m =0 the function $N_0 e^{-\sigma}$ and $N_1 (2-\sigma) e^{-\alpha/2}$, refers respec tively to the ground state (E_0) and first excited state (E_1) energy level if a variation function $N_3 (3-\sigma) e^{-\sigma/2}$ yield an average energy ε it will satisfy
(a) $\varepsilon \geq 0$ (b) $0 \leq \varepsilon \leq E_0$ (c) $\varepsilon \geq E_1$ (d) $E_0 \leq \varepsilon \leq E_1$

10. Consider the statements
(i) The energy calcualted by trial wave function in variational principle is always greater than or equal to zero
(ii) Variation principle is an alternative to Schrodinger Equation
Correct statements above is
(a) (ii) (b) (i) (c) (i), (ii) (d) None

11. Two trial wave function $\Phi_1 = (C_1 X)(a-x)$ and $\Phi_2 = C_1 x(a-x) + C_2 X^2 (a-x)^2$ give ground state energies E_1 and E_2 respectively, for the microscopic particle in a 1D box by using the variation method. If the exact ground state energy is E0 , the correct relationship between E_0,E_1 and E_2 are
(a) $E_0 = E_1 = E_2$ (b) $E_0 < E_1 < E_2$ (c) $E_0 < E_2 < E_1$ (d) $E_0 > E_2 = E_1$

12. A particle in 1D box (Potential energy V =0 inside the box between 0 to a, V = infinite outside) has the ground state energy $E_0 = (0.125\ h^2/ml^2)$ The expectation value of the above Hamiltonian with $\phi(x) = x(x-a)$ yields an energy E_1 Using a linear combination of two even function x(x-a) and X^2 $(x-a)^2$, we obtain the variational minimum to the ground state energy as E_2 the relationship between E_0 E_1 and E_2 respectively are
(a) $E_0 < E_1 < E_2$ (b) $E_0 < E_2 < E_1$ (c)$E_1 < E_0 < E_2$ (d)$E_2 < E_0 < E_1$

13. A trial function used in the variational method for the hydrogen atom had the form $\psi \exp^{(-r)} + C_2 \exp^{(-r/2)}$ From a variational procedure we obtained
(a) $c_1 = c_2 = 0$ (b) $c_1 = c_2 = 0$ (c) $c_1 = 0, c_2 = 1$ (d) $c_1 = 1, c_2 = 1$

14. Choosing some Hamiltonian H and an orthonormal basis, a linear variationis carried out to get approximate energy E_1. With 2 basis function can obtain $E_1(2) \leq E_2(2)$. Taking 3 basis function, similarly three ordered energies $E_1(3) \leq E_2(3) \leq E_3(3)$ are found. The relation which hold the good from the following is

(a) $\bar{E}_1(2) \le \bar{E}_1(3); \bar{E}_2(2) \le \bar{E}_2(3)$ (b) $\bar{E}_1(3) \le \bar{E}_1(2); \bar{E}_2(2) \le \bar{E}_2(3)$

(c) $\bar{E}_1(2) \le \bar{E}_1(3); \bar{E}_2(3) \le \bar{E}_2(2)$ (d) $\bar{E}_1(3) \le \bar{E}_1(2); \bar{E}_2(3) \le \bar{E}_2(2)$

15. The linear variation method using two orthogonal basic wavefunction, the two roots obtained are ε_0 and ε_1 $(\varepsilon_0 < \varepsilon_1)$ the correct relation of these with exact ground and first excited energies, $_0E$ and E_1, respectively are

(a) $\varepsilon_0 \ge E_0$ and $\varepsilon_1 < E_1$ (b) $\varepsilon_0 < E_1$ and $\varepsilon_1 \ge E_0$

(c) $\varepsilon_0 < E_0$ and $\varepsilon_1 \ge E_1$ (d) $\varepsilon_0 \ge E_0$ and $\varepsilon_1 \ge E_1$

QUANTA POINT

DPP- (17) Quantum Chemistry

1. A trial wave function of a system is expanded as $\psi_1 = C_1\Phi + C_2\Phi_2$. The matrix element of the Hamiltonian $<\Phi_1 H\Phi_1 = 0, <\Phi_1 H\Phi_2 >=<\Phi\,\Phi_2 H_1 >$ are 2.0 and $<\ \Phi\ _1 H\ \Phi\ _2\ > =\ 3\ .0\ $. The approximate ground state energy of the system from the linear variation principle is

   (a) -1.0 (b) -2.0 (c) +4.0 (d) +5.0

2. Given a wave function $\psi_1 = C_1\Phi_1 + C_2\Phi_2$ and the Hamiltonian matrix element as $\int \varphi_1 H\varphi_1 dv = 0 \int \varphi_1 H\varphi_2 dv = 2.5 \int \varphi_1 H\varphi_2 dv = 12.0,$ The variatonally determined ground state energy is

   (a) -0.52 (b) -0.50 (c) 12.50 (d) 12.52

3. The root of determinant in case of ethylene molecule in Huckel theory is

   (a) $\alpha+\beta, \alpha-\beta$ (b) $\alpha+2\beta, \alpha-\beta$ (c) $\alpha+2\beta, \alpha-2\beta$ (d) $\alpha+\beta, \alpha-2\beta$

4. The energy level for cyclobutadiene $\alpha+2\beta, \alpha, \alpha$ and $\alpha-2\beta$. The delocalization energy in this molecule is

   (a) 0 (b) -4β (c) -8β (d) 4α

5. Huckle Molecular orbital theroy can be applied to radical $CH_2 = CH - CH_2$

   (i) The secular determinant (where α, β and E have their usual meaning) is given by

   (a) $\begin{vmatrix} \alpha-E & \beta & 0 \\ \beta & \alpha-E & \beta \\ 0 & \beta & \alpha-E \end{vmatrix}$ (b) $\begin{vmatrix} \alpha-E & 0 & 0 \\ 0 & \alpha-E & \beta \\ 0 & \beta & \alpha-E \end{vmatrix}$

   (c) $\begin{vmatrix} \alpha-E & \beta & 0 \\ \beta & \alpha-E & 0 \\ 0 & 0 & \alpha-E \end{vmatrix}$ (d) $\begin{vmatrix} \alpha-E & -\beta & 0 \\ -\beta & \alpha-E & -\beta \\ 0 & -\beta & \alpha-E \end{vmatrix}$

6. The energy for a single electron excitation in cyclopropenieum cation according to Huckel Theory

   (a) β (b) 2β (c) 3β (d) 4β

7. The resonance integral for benzene in the Huckel model is 75 KJ/mole the energy required for the transition from HOMO to LUMO and to the highest unoccupied MO respectively will be

   (a) 150 and 225 KJ/mole (c) 150 and 300 KJ mole

   (b) 75 and 150 KJ/mole (d) 75 and 225 KJ/mole

8. As per Huckel theory, π- electron energy of cyclobutadine are

   (a) $\alpha+2\beta, \alpha+\beta, \alpha-\beta, \alpha-2\beta$ (b) $\alpha+2\beta, \alpha-\beta, \alpha-\beta, \alpha-2\beta$

   (c) $\alpha+2\beta, \alpha, \alpha-2\beta$ (d) $\alpha+\beta, \alpha-\beta, \alpha-\beta, \alpha-2\beta$

9. The correct statement regarding cyclobutadine molecule is (If $\beta = -75$ KJ/mole)

QUANTA POINT

(a) It is diamagnetic in nature and energy required for the excitation is 75 KJ/mole

(b) It is a paramagnetic in nature and enegy required for the transition is 150 KJ/mole

(c) It is diamagnetic in nature and energy required for the excitation is 150 KJ/mole

(d) It is a paramagnetic in nature and energy required for the excitation is 75 KJ/mole

10. Consider the statement

(i) The concept of a bond formation energy is different than delocalization energy

(ii) The of π bond formation energy in benxene is 6β

(iii) The delocalization energy for cyclobutadiene molecule is zero

Correct statement above are

(a) (i), (ii) (b) (ii), (iii) (c) (i),(iii) (d) all

11. The electronic transition energy from $\pi_1\pi \rightarrow 2$ in propenyl radical is 4.8 eV. Within the frame work of Huckel theory, the transitions energy from $\pi_1\pi \rightarrow 3$ would be

(a) 2.4 eV (b) 4.8 eV (c)9.6 eV (d) 14.4 eV

12. Idenfity the huckel determinant for cyclobutadiene

(a) $\begin{vmatrix} \alpha-E & \beta & 0 \\ \beta & \alpha-E & \beta \\ 0 & \beta & \alpha-E \end{vmatrix}$ (b) $\begin{vmatrix} \alpha-E & \beta & 0 \\ 0 & \alpha-E & \beta \\ 0 & \beta & \alpha-E \end{vmatrix}$

(c) $\begin{vmatrix} \alpha-E & \beta & 0 \\ \beta & \alpha-E & 0 \\ 0 & \beta & \alpha-E \end{vmatrix}$ (d) $\begin{vmatrix} \alpha-E & -\beta & 0 \\ -\beta & \alpha-E & -\beta \\ 0 & -\beta & \alpha-E \end{vmatrix}$

13. Simple Hukel molecular orbital theory

(a) Consider electron-electron repulsion explicity

(b) Distinguish cis butadiene and cyclobutadiene

(c) Distinguish cis butadiene and trans butadiene

(d) Has different coulomb integral for non equivalent carobon.

14. Consider the statement

(i) Huckel molecular orbital theory is based on $\pi-\sigma$ seperability

(ii) The value of resonance energy generally remain in the form of resonance integral

(iii) The approximation of considering overlap integral zero in Huckel molecular orbital theory is a bad approximation.

The correct staement above are

(a) (i), (ii) (b) (ii), (iii) (c) (i), (iii) (d) all

15. True or false

(i) Huckel approximation is used to determine the energies and shpaes of the $\pi\pi$ molecular orbitals in conjugated systems.

(ii) All diagonal Hamilitionian integrals Hii are called Coulomb integrals and those of type HijHij are called resoance integrals.

(iii) Huckel Theory can be extended to address other types of atoms in conjugated molecules (e.g., nitrogen and oxygen).

QUANTA POINT

DPP- (18) Quantum Chemistry

1. The total bond order between adjacent carbon atom of benzen is
(a) 0.5 (b) 2.0 (c) 1.5 (d) 2.5

2. The Huckel Molecular Orbital of benzene that is degenerate with the molecular orbital (1/2)

$\left[\chi_2 + \chi_3 \chi_5 \chi_4\right]$

(a) $1/\sqrt{2}\,[2x_1+x_2-x_3-2x_4-x_5+x_6]$ (b) $1/\sqrt{2}\,[x_2-x_3+x_5-x_6]$
(c) $1/\sqrt{2}\,[2x_1-x_3-2x_4-x_5-x_6]$ (d) $1/\sqrt{2}\,[x_1-x_2+x_3-x_4+x_5-x_6]$

3. The highest energy p molecular orbital for the allyl system is

(a) $\frac{1}{\sqrt{2}}\chi_1 + \Gamma\chi_2 + \frac{1}{\sqrt{2}}\chi_3$ (b) $\frac{1}{\sqrt{2}}\chi_1 - \frac{1}{\sqrt{2}}\chi_3$

(c) $\frac{1}{\sqrt{2}}\chi_1 - \frac{1}{\sqrt{2}}\chi_2 + \frac{1}{2}\chi_3$ (d) $\frac{1}{\sqrt{2}}\chi_1 - \frac{1}{2}\chi_2 - \frac{1}{\sqrt{2}}\chi_3$

4. Consider the statement regarding stability of $H_3^+, H_3^- H_3$ is

(i) H_3^- is more stanle in linear configuration

(ii) H_3^- and H_3 is more stable in linear configuration

(iii) H_3^+ and H_3 is more stable in triangular configuration

(iv) H_3^+ and H_3 is more stable in triangular configuration

(a) (i) and (ii) (b) (i),(ii) and (iii) (c) (i)(iii) (d) (iii) ,(iv)

5. Free valence index corresponding to central atom carbon atom in allyl cation is
(a) 1.02 (b) .732 (c) .32 (d) .52

6. The energy levels of cyclopropene are The delocalization energy in $C_3 H_3$ is
(a) 2β (b) 0 (c) β (d) 3β

7. For a one-dimensional (x) harmonic oscillator perturbed by an x^3 potential, the sum of the first order and second order correction to the ground state energy is
(a) < 0 (b) 0 (c) > 0 (d) ≥ 0

8. A particle in one D box of length 2a with potential energy

$$v = \begin{cases} 0 & |x| < a \\ \infty & |x| > a \end{cases}$$

is perturbed by a potential V'=c. eV where c is constant, First order correction in excited state of the system is

QUANTA POINT

(a) 0 (b) 5 (c) ∞ (d) 10

9. Difference of average value of position x for state n = 1 and n = 2 of a particle confined to move in 1 D box of length L is

(a) L/4 (b) L/3 (c) L/2 (d) 0

10. The Hermitian operator among the following is

(a) $i\hbar\frac{d^2}{dx^2}$ (b) $-i\hbar\frac{d^1}{dx}$ (c) $i\hbar x$ (d) $i\hbar$

11. One of the Huckel Molecular orbital of 1, 3 Butadiene is

$\varphi = 0.60\chi_1 + 0.37\chi_2 - 0.37\chi_3 - 0.60\chi_4$

The energy of this orbital in terms of Coulomb (α) and Reasonce (β) integrals are

(a) $\alpha + 1.62$ (b) $\alpha + 6.2$ (c) $\alpha - 1.62$ (d) $\alpha - 6.2$

12. While the vibrational energy of an osicllator in v = 0 (ground state) is non-zero, the rotational energy of a rigid rotor in J = 0 state (ground state) can be zero. Pick the correct answer

(a) Vibrational energy of an oscillator consists of both potential as well as kinetic energy of a whereas the rotational energy of the rotor has only the kinetic energy

(b) It is a rigid rotor

(c) Vibrational and rotational degree of freedom is decoupled from each other

(d) None of the above

13. For a one dimensional quantum mechanical harmonic osicllator

(a) Average linear momentum is non zero average displacement is zero

(b) Average linear momentum is zero average displacement is zero

(c) Average linear momentumis zero average displacement is non zero

(d) Average linear momentum and average displacement both are non zero

14. The wavefunction correspondign to energy level $\alpha + 1.618\beta$ in case of butadience molecule according to HMO is

(a) $\psi = 0.3755(\chi_1 + \chi_4) + 0.6070(\chi_2 + \chi_3)$ (b) $\psi = 0.3070(\chi_1 - \chi_4) + 0.3755(\chi_2 - \chi_3)$

(c) $\psi = 0.6070(\chi_1 + \chi_4) - 0.3755(\chi_2 + \chi_3)$ (d) $\psi = 0.3755(\chi_1 - \chi_4) - 0.6070(\chi_2 - \chi_3)$

15. The energy level corresponding to wavefunction

$\psi = 0.5(\chi_1 + \chi_3) - 0.707\chi_2$

of allyl system (cation, anion or radical) according to HMO is

(a) $\alpha + 1.414\beta$ (b) $\alpha - 1.414\beta$ (c) α (d) $\alpha - 414\beta$

QUANTA POINT

DPP- (19) Quantum Chemistry

1. If $\psi = 0.8\,\Phi_A + 0.4\,\Phi_B$ is a normalized molecular orbital of a diatomic molecule AB constructed from Φ_A and Φ_B which are also normalised, then the overlap integral between Φ_A and Φ_B is

   (a) 0.11 (b) 0.31 (c) 0.51 (d) 0.71

2. One molecular orbital of polar molecule AB has the form $C_A\psi_A + C_B\psi_B$ where ψ_A and ψ_B are normalised atomic orbital of centred on A and B respectively. The electron in this orbital is found on atom B with a probability of 90%. Neglecting the overlapping integral between ψ_A and Ψ_B, a possible set of C_A and C_B are

   (a) $C_A = 0.95$, $C_B = 0.32$ (b) $C_A = 0.10$, $C_B = 0.90$

   (c) $C_A = -0.95$, $C_B = 0.32$ (d) $C_A = 0.32$, $C_B = 0.95$

3. In a molecule XY, let ψ_x and ψ_y denote normalized atomic orbital of atom X and Y, respectively. A normalized molecular orbital of XY is given by $\psi_+ = 0.56\,(\psi_x + \psi_y)$. The value of overlap integral of ψ_x and ψ_y is …. (Up to two decimal places)

   (a) 0.5 (b) 1.0 (c) 1.5 (d) 2.0

4. The lowest energy normalized wave function of H_2^+ molecule (r_1 and r_2 are the distance between the electron and nuclei 1 and 2 respectively

   (a) $\psi = \left(e^{-r_1/a_0} + e^{-r_2/a_0}\right)$ (b) $\psi = \left(e^{-r_1/a_0} - e^{-r_2/a_0}\right)$

   (c) $\psi = e^{-r_1/a_0}$ (d) $\psi = e^{-r_2/a_0}$

5. Determine the normalization constant for $\{\Phi_a(1)\,\Phi_b(2) + \Phi_a(2)\,\Phi_b(1)\}$ for a homonuclear diatomic molecule according to valence bond theory. If $S = 0.59$.

   (a) 0.30 (b) 0.60 (c) 1 (d) 0.90

6. The simultaneous configuration of angular momentum operator L^2 and L_z, are

   (a) All of 2s, $2p_x$, $2p_y$ and $2p_z$ orbital (b) all of 2s, $2p_x$, $2p_y$

   (c) only 2s and $2p_z$ (d) Only $2p_z$

7. The wavefunction of a diatomic molecule has the form $\psi = 0.89\,\Phi_{covalent} + 0.45\,\Phi_{ionic}$ the chance that both electron will be found on the same atom out of hundred inspection of the molecule approximately are

   (a) 79 (b) 20 (c) 45 (d) 60

QUANTA POINT

8. In the formation of H_2 molecule from 2H atoms placed at position A and B and separated by a distance r_{AB}, a part of spatial wave function is $\Phi_A(1)\,\Phi_A(2) + \Phi_B(1)\Phi_B(2)$

(a) This is covalent term and is important as $r_{AB} \to$ infinite

(b) This is ionic term and is important as $r_{AB} \to$ infinite

(c) This is covalent term and is important as $r_{AB} \to 0$

(d) This is ionic term and is important as $r_{AB} \to 0$

9. Consider the statements

(i) Overlapping S_{ab} can have value between zero and one. In order to have a chemical bond it is necessary that $S_{ab} > 0$.

(ii) The bonding orbital change sign on inversion in p_x and p_y orbital so it is ungerade, and antibonding orbital remain same on inversion so it is gerade.

(iii) Bonding orbital show a build up an electron density in an internuclear region while antibonding orbital show a decrease of electron density in internuclear region.

Correct statements above is/are

(a) (i), (ii) (b) (ii), (iii) (c) (i), (ii), (iii) (d) none

10. In simple molecular orbital theory of hydrogen molecular bonding σ_g and ant bonding σ_u molecular orbitals are constructed as linear combinations of atomic orbitals of two hydrogen atoms. The spatial part of a purely covalent singlet wavefunction is obtained by

(a) $\sigma_g^2 + \sigma_u^2$ (b) σ_g^2 (c) $\sigma_g^2 - \sigma_u^2$ (d) $\sigma_g^2 + (1/2)\sigma_u^2$

11. The spatial part of hydrogen molecular wavefunction in simplest molecular orbital theory is given by σ_g^2 where σ_g is a normalized linear combination of two hydrogen 1s orbitals. Which of the following is true about the wave function?

(a) It contains only covalent terms

(b) It includes only a small amount of ionic terms

(c) It contains only ionic terms

(d) It over estimates the ionic terms

12. The two limiting wave function of the ground state of H_2^+ molecular ion, as the intermediate separation goes to (i) infinity (ii) zero (0) are $\{1S_n, 1S_b$ are 1S - orbital wave function of H atom a and b in H_2^+ molecule and $1S_{He}$ is the wavefunction of 1S orbital of $He^+\}$

(a) (i) $1s_a(r)$; (ii) $1s_a(r)$

QUANTA POINT

(b) (i) $1s_b(r)$; (ii) $1s_a(r)$

(c) (i) $1s_a(r_1)\,1s_b(r_2)$; (ii) $1s_{He}(r_1)\,1s_{He}(r_2)$

(d) (i) $1s_a(r) + 1s_b(r)$; (ii) $1s_{He}(r)$

13. Consider the statements

(i) Every H_2^+ Eigen functions is either gerade (i.e., symmetric for inversion) or ungerade.

(ii) The continuity of symmetry enables the σ_g state of H_2^+ to correlate with an s-type AO of He^+ as R goes to zero.

(iii) At R = 0 because the σ_u state of H_2^+ correlates with a 2p AO of He^+.

The correct statements above is/are

(a) (i) (b) (i), (ii) (c) (i), (ii), (iii) (d) none

14. A molecular orbital of a diatomic number molecule changes sign when it is rotated by 180° around the molecular axis

(a) π (b) σ (c) δ (d) Φ

15. Correct combination for π and π^* orbitals in B_{-2}- molecule is

π	π^*
(a) Gerade	Ungerade
(b) Ungerade	Gerade
(c) Gerade	Gerade
(d) Ungerade	Ungerade

QUANTA POINT

DPP- (20) Quantum Chemistry

1. The value of $[s_x, s_y]$ is equal to

   (a) $2\,i\,s_z$ (b) $-2\,i\,s_z$ (c) $i\,s_z$ (d) $-i\,s_z$

2. The value of $S_x^2 S_y S_z^2$ is equal to

   (a) $(h/4p)^5\,s_z$ (b) $(h/4p)^3\,s_Y$ (c) $(h/4p)^5\,s_Y$ (d) $(h/4p)^3\,s_z$

3. The spin angular momentum operator S_Z in form of Pauli matrix is

   (a) $h\,s_z / 2p$ (b) $h\,s_z / 4p$ (c) $-h\,s_z / 2p$ (d) $-h\,s_z / 4p$

4. For two atom two electron system, if we operate the total spin angular momentum operator S^2 on function {a(1) b (2) - b (1) a (2)}. The corresponding eigenvalue is

   (a) $h^2 / 2p^2$ (b) $h/ 2p$ (c) 0 (d) h^2

5. The value of $s_x\, s_Y\, s_z$ is equal to

   (a) 1 (b) i (c) -i (d) -1

6. For H_2 molecule, the ground state wave function $y(1, 2) = F(1, 2)\, s(1, 2)$ where F refers to the space part and s refers to spin part, given that $F(1, 2) = F(2, 1)$, the form s (1, 2) will be

   (a) a (1) b (2) (b) a (2) b (1)

   (c) {a (1) b (2) - b (1) a (2)} (d) {a (1) b (2) + b (1) a (2)}

7. An excited triplet state wave function of hydrogen molecule with the electronic configuration $\sigma_g^1\ \sigma_u^1$ has the following space part

   (a) $\sigma_g(1)\,\sigma_u(2)$ (b) $\sigma_g(1)\,\sigma_u(2) + \sigma_u(1)\,\sigma_g(2)$

   (c) $\sigma_g(1)\,\sigma_u(2) - \sigma_u(1)\,\sigma_g(2)$ (d) $\sigma_g(1)\,\sigma_u(2) + \sigma_u(1)\,\sigma_u(2)$

8. For H_2 molecule in the excited state the spin part of triplet state with $m_s = 0$ is proportional to

   (a) a (1) b (2) (b) a (2) b (1)

   (c) {α (1), β (2) - β (1) α (2)} (d) {α (1) β (2) + β (1) α (2)}

QUANTA POINT

9. The spatial part of wave function of the atom in its ground state is 1s(1) 1s(2) the spin part of the wave function would be

(a) $\alpha(1)\,\alpha(2)$ (b) $\beta(1)\,\beta(2)$

(c) $(1/\sqrt{2})\,\{\alpha(1)\,\beta(2) - \beta(1)\,\alpha(2)\}$ (d) $(1/\sqrt{2})\,\{\alpha(1)\,\beta(2) + \beta(1)\,\alpha(2)\}$

10. Which of the following statement is incorrect?

(a) A slater determinant is an antisymmetric wave function.

(b) Electronic wave function should be represented by Slater determinant.

(c) A slater determinant always corresponding to particular spin state.

(d) A slater determinant obey the Pauli exclusion principle

11. For n e^- atom the normalization constant for Slater Determinant is

(a) $1/(N)^{1/2}$ (b) $1/(N!)^{1/2}$

(c) $1/(N)^{1/2}$! (d) $1/(2N!)^{1/2}$

12. A slater determinant corresponding to ionic part of ground state valence band wave function of H_2 molecules is [{$1S_a\alpha$, $1S_a$, $1S_b\alpha$, $1S_b\beta$,} are atomic spin orbital of hydrogen atom a and b of hydrogen molecule

(a) $\begin{vmatrix} 1s_a\alpha(1) & 1s_a\beta(1) \\ 1s_a\alpha(2) & 1s_a\beta(2) \end{vmatrix}$ (b) $\begin{vmatrix} 1s_a\alpha(1) & 1s_b\beta(1) \\ 1s_a\alpha(2) & 1s_b\beta(2) \end{vmatrix}$ (c) $\begin{vmatrix} 1s_a\alpha(1) & 1s_b\alpha(1) \\ 1s_a\alpha(2) & 1s_b\alpha(2) \end{vmatrix}$ (d) $\begin{vmatrix} 1s_a\alpha(1) & 1s_b\beta(1) \\ 1s_a\alpha(1) & 1s_b\beta(2) \end{vmatrix}$

13. Which of these are not a suitable unnormalized wave function for excited state $1S^1 2S^1$ electron configuration of the helium atom

(a) [1s(1)2s(2)-2s(1)1s(2)][β(1)β(2)] (b) [1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)-β(1)α(2)]

(c) [1s(1)2s(2)-2s(1)1s(2)] (d) [1s(1)2s(2)+2s(1)1s(2)][α(1)β(2)]

14. A satisfactory spin wave function for an excited helium atom is

(a) $\frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \alpha(2)\beta(1)]$ (b) $\alpha(1)\beta(2)$ (c) $\frac{1}{\sqrt{2}}[\alpha(1)\alpha(2) + \beta(1)\beta(2)]$ (d) $\alpha(2)\beta(1)$

15. If where and are spin angular momentum operators and $|\alpha>$ is spin up Eigen function, then the value of 'a' is _____ (Round off to one decimal place)

(a) 0.5 (b) 0.2 (c) 0.3 (d) 0.1

QUANTA POINT

DPP- 1 To 20 QUANTUM CHEMISTRY

ANSWER KEY

DPP-1

1.	(b)	2.	(d)	3.	(d)	4.	(c)	5.	(d)	6.	(c)	7.	(b)
8.	(d)	9.	(d)	10.	(c)	11.	(a)	12.	(b)	13.	(a)	14.	(c)
15.	(d)												

DPP-2

1.	(d)	2.	(c)	3.	(c)	4.	(b)	5.	(a)	6.	(b)	7.	(b)
8.	(b)	9.	(c)	10.	(c)	11.	(d)	12.	(a)	13.	(c)		

DPP-3

1.	(b)	2.	(b)	3.	(b)	4.	(b)	5.	(c)	6.	(d)	7.	(b)
8.	(c)	9.	(c)	10.	(b)	11.	(c)	12.	(d)	13.	(c)	14.	(b)
15.	(a)												

DPP-4

1.	(a)	2.	(c)	3.	(c)	4.	(c)	5.	(b)	6.	(c)	7.	(d)
8.	(c)	9.	(d)	10.	(c)	11.	(a)	12.	(b)	13.	(c)	14.	(b)
15.	(d)												

DPP-5

1.	(b)	2.	(a)	3.	(c)	4.	(b)	5.	(c)	6.	(b)	7.	(b)
8.	(b)	9.	(b)	10.	(c)	11.	(c)	12.	(b)	13.	(c)	14.	(d)
15.	(b)	16.	(b)	17.	(c)	18.	(d)	19.	(b)	20.	(c)		

DPP-6

1.	(c)	2.	(b)	3.	(d)	4.	(a)	5.	(d)	6.	(b)	7.	(d)
8.	(c)	9.	(c)	10.	(b)	11.	(d)	12.	(b)	13.	(c)	14.	(a)
15.	(d)												

QUANTA POINT

DPP-7

1. (c) 2. (c) 3. (b) 4. (c) 5. (c) 6. (a) 7. (b)
8. (d) 9. (c) 10. (a)

DPP-8

1. (a) 2. (c) 3. (d) 4. (c) 5. (d) 6. (a) 7. (c)
8. (c) 9. (c,d,c) 10. (a) 11. (c) 12. (a) 13. (a) 14. (c)
15. (c)

DPP-9

1. (c) 2. (d) 3. (a) 4. (b) 5. (c) 6. (a) 7. (c)
8. (b) 9. (a) 10. (c) 11. (a) 12. (b) 13. (d) 14. (b)
15. (d)

DPP-10

1. (c) 2. (a) 3. (b) 4. (a) 5. (d) 6. (b) 7. (b)
8. (c) 9. (b) 10. (b) 11. (c) 12. (c) 13. (c) 14. (c)
15. (a)

DPP-11

1. (b) 2. (c) 3. (a) 4. (d) 5. (d) 6. (c) 7. (d)
8. (a) 9. (b) 10. (c) 11. (b) 12. (c) 13. (c) 14. (c)
15. (a)

DPP-12

1. (c) 2. (c) 3. (c) 4. (b) 5. (c) 6. (b,c) 7. (d)
8. (a,c) 9. (b) 10. (a) 11. (b) 12. (c) 13. (d) 14. (a)
15. (b)

DPP-13

1. (a) 2. (a) 3. (a) 4. (a) 5. (a) 6. (c) 7. (c)
8. (c) 9. (d) 10. (d) 11. (a) 12. (d) 13. (a) 14. (d)
15. (b)

DPP-14

1. (d) 2. (a) 3. (d) 4. (a) 5. (b) 6. (d) 7. (b)
8. (b) 9. (c) 10. (a) 11. (d) 12. (b) 13. (a) 14. (c)

QUANTA POINT

DPP-15

1.	(c)	2.	(d)	3.	(c)	4.	(b)	5.	(a)	6.	(b)	7.	(c)
8.	(d)	9.	(b)	10.	(c)	11.	(a)	12.	(a)	13.	(d)	14.	(a)
15.	(c)												

DPP-16

1.	(a)	2.	(b)	3.	(a)	4.	(b)	5.	(b)	6.	(b)	7.	(b)
8.	(d)	9.	(c)	10.	(a)	11.	(c)	12.	(b)	13.	(b)	14.	(d)
15.	(d)												

DPP-17

1.	(a)	2.	(b)	3.	(a)	4.	(a)	5.	(a)	6.	(c)	7.	(a)
8.	(c)	9.	(b)	10.	(c)	11.	(c)	12.	(c)	13.	(b)	14.	(d)
15.	(a,b,c)												

DPP-18

1.	(c)	2.	(a)	3.	(c)	4.	(d)	5.	(c)	6.	(a)	7.	(a)
8.	(a)	9.	(d)	10.	(b)	11.	(b)	12.	(a)	13.	(b)	14.	(a)
15.	(c)												

DPP-19

1.	(a)	2.	(c)	3.	(b)	4.	(c)	5.	(d)	6.	(c)	7.	(c)
8.	(d)	9.	(c)	10.	(c)	11.	(b)	12.	(a)	13.	(d)	14.	(a)
15	(a)												

DPP-20

1.	(a)	2.	(c)	3.	(b)	4.	(c)	5.	(d)	6.	(c)	7.	(c)
8.	(d)	9.	(c)	10.	(c)	11.	(b)	12.	(a)	13.	(d)	14.	(a)
15.	(a)												

QUANTA POINT